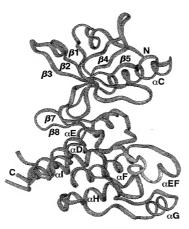
# FIG. 1a

	1/67		
863 509 1025 856 622	923 568 1083 916 681	953 586 1095 946 741	1010 605 1114 1004 800
nucleotide-binding loop (2007)  VEGF-R2 806 MDPDELPLDEHCERLPYDASKWEFPRDRLKLGK PLGRGAFGQVEADAFGIDKTATCR	VEGF-R2 864 TVAVKMLKEGATHSEHRALMSELKILIHIGHHLNVVNLLGACTKPGGPLMVIVEFCKFGN FGFR1 510 KVAVKMLKEGATHSENDLSEMSMMKKMIGKHKNIINLGACT-DODELYVIVEY ASKGN IRK 1026 RVAVKTVNESASLRENIEFLNESVMKGFTCH-HVVRLLGACT-DODELYVIVEY ASKGN PVEGF-R1 837 TVAMKMLKGGATASEFKALMTELKILTHIGHHLNVNNLLGACTKGGGPLMVIVEY CKYGN PDGFFR	VEGF-R2 924 ISTYLRSKRNEFVPYKTKGARFRQGKDYVG-FGFR1 569 LRSTLQARRPPGLEYCYN-FGFR1 1084 LKSVTRSLRPEA-FGFRN-FVFRKKME-FVFRKKME-FWFKKKELDIFGLNPADESTRSYVILSFENNGDYMDMKQADTTQ	VEGF-R2 954AIPVDLKRRLDS1TSSQSSASSGFVEEKSLSDVEEEEAPEDLYKDFLTLEHLICYSF FGFR1 587

## FIG. 1b

	2/67	
1070 665 1174 1064 860	923 568 1083 916 681	1171 765 1274 1165 961
vegF- R2 1011 QVAKGMEFDLASRKC IHRDLAARN I LLSE KNVKICDFGLARDI Y K DPDYVRKGDA RL PLK FGFR1 606 QVARGMEFDLASRKC I HRDLAARNVL Y TEDNINWKIADFGLARDI HI DY Y KK TYNGR LP PK 1115 E I ADGAMPY - LNAKKFC Y HRDLAARN LY TEDNING DFGAMTRDI Y ETDY YR KGGKG ILL PN V KGF- R1 1005 QVARGMIFDLASRKC I HRDLAARN I LLSENNV KI DDFGLARDI Y KNPDYVRKGGKG ILL PN PDGFRα 801 QVARGMEFL-LASKKC I HRDLAARN V LAQGKI I VKI DDFGLARDI MHDSN YV SKGST FL PV K	VEGF-R2 1071 WMAPETI FDRVYTLQSDVWSFGVLLWEIFSLGASPYPGVK I DEJECRRLKEGTRMRRAPDY FGFR 1 1071 WMAPEALFDR I YTHOSDVWSFGVLLWEIFSLGGSPYPGSPYDEEF-KLLKEGHRWDRRPSN I RT 1775 WMAPEALFDR I YTHOSDVWSFGVLLWEIFSLGGSPYDGUS NEOVIL KFVMDG9′L LDLQPDN I RT 1175 WMAPESI FDK I YSTK SDVWSYGVLLWEIFSLGGSPYPGVQMDEDFCSRLREGMRNRRAPEY PDGFRα 861 WMAPESI FDN LYTTLSDVWSYGI LLWEIFSLGGSPYPGVQMDEDFCSRLREGMRNRRAPEY PDGFRα	νEGF-R2 1131 TTPEMYOTMLDCWHGEPSORP FSELVEHIGNLLQANAQQD FGFR1 725 CTNELYMMMRDCWHAVPSORPTFKQLVEDLDRIVA.I TSNQE IRK 1234 CPERYTYDLMRMKOWGNNNMRPTELEIVLLRDDLHPSFPEV FYEGF-R1 1125 STPEIYQIMLDCWHRDFRERPELVEKLGDLQANVQQD PDGFRα 1921 ATSEVYEIMVKCWNSEPEKRPSFYHLSEIVENLPGQYKKS

#### FIG. 2a



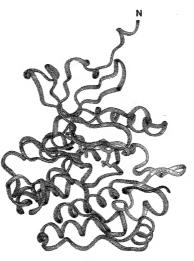
VEGFR2D50P

FIG. 2b

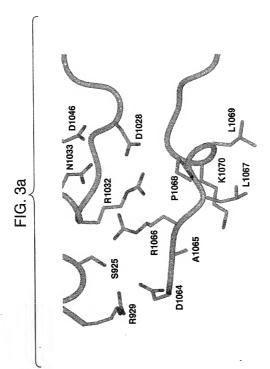


FGFR1

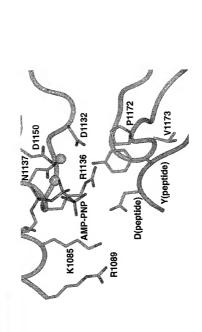


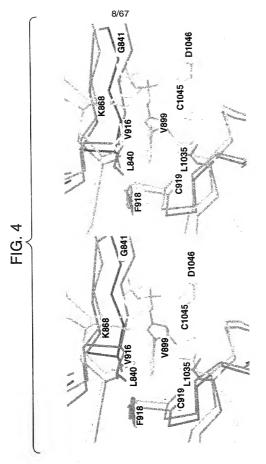


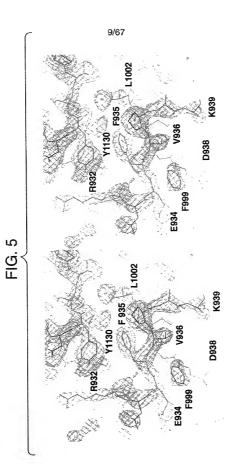
IRKP

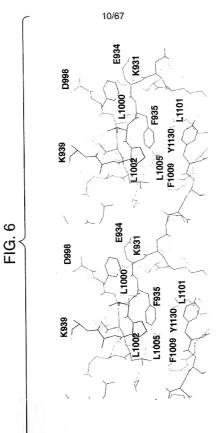












#### FIG. 7(1)

ATOM 1 CB LEU 820 49.908 45.905 17.938 1.00 48.95 **ATOM** 2 CG LEU 820 50.568 45.069 16.833 1.00 43.57 ATOM 3 CD1 LEU 820 50,004 45,358 15,456 1,00 43,59 ATOM 4 CD2 LEU 820 52,066 45,345 16,886 1,00 47,45 ATOM 5 C LEU 820 49.216 48.321 17.530 1.00 48.14 6 O LEU 820 ATOM 48.196 48.587 18.187 1.00 52.58 9 N LEU 820 50.481 47.725 19.581 1.00 53.68 ATOM 11 CA LEU 820 50.302 47.387 18.117 1.00 50.63 **ATOM** 12 N PRO 821 49,435 48,842 16,306 1,00 41,32 ATOM 50.680 48.870 15.520 1.00 45.54 **ATOM** 13 CD PRO 821 ATOM 14 CA PRO 821 48,465 49,733 15,700 1,00 31,06 ATOM 15 CB PRO 821 49,067 49,985 14,352 1,00 28,89 16 CG PRO 821 50.509 50.148 14.734 1.00 43.44 ATOM ATOM 17 C PRO 821 47.123 49.165 15.569 1.00 26.14 18 O PRO 821 46.948 47.970 15.374 1.00 26.03 ATOM ATOM 19 N TYR 822 46.154 50.024 15.776 1.00 16.25 ATOM 21 CA TYR 822 44,799 49,643 15,582 1.00 18.88 ATOM 22 CB TYR 822 44,061 49,519 16,916 1.00 17,42 23 CG TYR 822 42.584 49.316 16.728 1.00 18.46 ATOM ATOM 24 CD1 TYR 822 41.674 50.341 17.047 1.00 21.12 25 CE1 TYR 822 40.314 50.206 16.812 1.00 13.80 **ATOM** ATOM 26 CD2 TYR 822 42.086 48.144 16.175 1.00 12.24 ATOM 27 CE2 TYR 822 40.714 47.997 15.951 1.00 13.44 ATOM 28 CZ TYR 822 39.838 49.028 16.268 1.00 14.38 ATOM 29 OH TYR 822 38,480 48,887 16,073 1,00 19,73 ATOM 31 C TYR 822 44,253 50,760 14,705 1,00 16,93 32 O TYR 822 ATOM 44,172 51,904 15,112 1,00 20,70 ATOM 33 N ASP 823 44,054 50,456 13,439 1,00 15,20 35 CA ASP 823 ATOM 43.509 51.418 12.506 1.00 13.55 43.856 50.945 11.091 1.00 11.37 ATOM 36 CB ASP 823 ATOM 37 CG ASP 823 43,456 51,933 10,016 1,00 16,45 42.546 52.754 10.258 1.00 21.86 ATOM 38 OD1 ASP 823 ATOM 39 OD2 ASP 823 44.022 51.854 8.904 1.00 12.33 ATOM 40 C ASP 823 41.983 51.489 12.738 1.00 14.14 ATOM 41 O ASP 823 41.224 50.722 12.172 1.00 19.73 ATOM 42 N ALA 824 41.539 52.415 13.572 1.00 11.88 40.126 52.554 13.876 1.00 14.80 39.928 53.610 14.973 1.00 12.02 44 CA ALA 824 ATOM ATOM 45 CB ALA 824 39.259 52.893 12.658 1.00 19.09 ATOM 46 C ALA 824 ATOM 47 O ALA 824 38.062 52.610 12.641 1.00 23.54

#### FIG. 7(2)

ATOM 48 N SER 825 39.857 53.496 11.635 1.00 18.25 ATOM 50 CA SER 825 39.118 53.867 10.450 1.00 12.65 ATOM 51 CB SER 825 40.023 54.678 9.543 1.00 11.88 ATOM 52 OG SER 825 39.315 55.003 8.370 1.00 20.94 38.669 52.594 9.746 1.00 12.30 ATOM 54 C SER 825 37.543 52.461 9.317 1.00 14.94 ATOM 55 O SER 825 56 N LYS 826 39,557 51,633 9,642 1,00 14,98 ATOM 58 CA LYS 826 39,188 50,396 8,988 1,00 22,45 ATOM 59 CB LYS 826 40.445 49.660 8.483 1.00 16.46 ATOM 40,091 48,370 7.820 1.00 23.00 ATOM 60 CG LYS 826 40.962 48.071 6.657 1.00 26.19 ATOM 61 CD LYS 826 42,391 48,041 7,092 1,00 35,70 ATOM 62 CE LYS 826 63 NZ LYS 826 43,272 48,003 5,891 1,00 40,17 ATOM 67 C LYS 826 38.324 49.437 9.839 1.00 21.47 ATOM 68 O LYS 826 37.363 48.850 9.336 1.00 22.56 ATOM 69 N TRP 827 38.589 49.376 11.144 1.00 20.96 ATOM ATOM 71 CA TRP 827 37,917 48,406 11,996 1,00 16,87 38,974 47,620 12,785 1,00 18,53 ATOM 72 CB TRP 827 73 CG TRP 827 39,942 46,898 11,910 1,00 12,95 ATOM 74 CD2 TRP 827 39,643 45,810 11,029 1,00 9,73 ATOM 75 CE2 TRP 827 40.795 45.562 10.274 1.00 9.36 ATOM 76 CE3 TRP 827 38.505 45.038 10.801 1.00 11.54 ATOM ATOM 77 CD1 TRP 827 41,233 47,231 11,684 1,00 12,87 ATOM 78 NE1 TRP 827 41.753 46.440 10.689 1.00 10.49 ATOM 80 CZ2 TRP 827 40.848 44.565 9.299 1.00 12.36 ATOM 81 CZ3 TRP 827 38.556 44.053 9.826 1.00 10.55 39,718 43,830 9,087 1,00 11,88 ATOM 82 CH2 TRP 827 ATOM 83 C TRP 827 36.830 48.795 12.953 1.00 17.75 35.985 47.951 13.271 1.00 15.08 **ATOM** 84 O TRP 827 ATOM 85 N GLU 828 36.855 50.043 13.416 1.00 16.92 ATOM 87 CA GLU 828 35.908 50.518 14.413 1.00 19.52 ATOM 88 CB GLU 828 36,289 51,920 14,885 1,00 17,10 89 CG GLU 828 35.581 52,363 16,148 1,00 12,70 ATOM 90 CD GLU 828 36.106 51.707 17.400 1.00 21.57 ATOM 91 OE1 GLU 828 37.219 51.118 17.386 1.00 21.15 ATOM ATOM 92 OE2 GLU 828 35,402 51.819 18.426 1.00 22.43 93 C GLU 828 34.494 50.510 13.910 1.00 20.94 ATOM 34.245 51.024 12.818 1.00 26.92 94 O GLU 828 ATOM 95 N PHE 829 33,569 49,990 14,734 1.00 21,12 **ATOM** 97 CA PHE 829 32.138 49.880 14.391 1.00 17.93 ATOM 31,791 48,400 14,160 1.00 16,42 **ATOM** 98 CB PHE 829 99 CG PHE 829 30,384 48,164 13,669 1,00 20,17 ATOM

## FIG. 7(3)

	(-)	
ATOM	100 CD1 PHE 829	30.020 48.484 12.363 1.00 21.31
ATOM	101 CD2 PHE 829	29.415 47.612 14.516 1.00 23.04
ATOM	102 CE1 PHE 829	28.712 48.254 11.921 1.00 18.76
ATOM	103 CE2 PHE 829	28.093 47.375 14.071 1.00 15.20
ATOM	104 CZ PHE 829	27.750 47.692 12.792 1.00 17.17
ATOM	105 C PHE 829	31.310 50.495 15.533 1.00 14.65
ATOM	106 O PHE 829	31.574 50.211 16.686 1.00 16.15
ATOM	107 N PRO 830	30.270 51.298 15.224 1.00 13.29
ATOM	108 CD PRO 830	29.707 51.633 13.901 1.00 11.63
ATOM	109 CA PRO 830	29.481 51.918 16.292 1.00 14.76
ATOM	110 CB PRO 830	28.636 52.948 15.565 1.00 13.82
ATOM	111 CG PRO 830	28.414 52.364 14.252 1.00 14.42
ATOM	112 C PRO 830	28.629 51.005 17.098 1.00 19.79
ATOM	113 O PRO 830	27,750 50,339 16,562 1.00 26,60
ATOM	114 N ARG 831	28.830 51.060 18.410 1.00 18.39
ATOM	116 CA ARG 831	28.085 50.246 19.335 1.00 14.56
ATOM	117 CB ARG 831	28.469 50.580 20.743 1.00 11.53
ATOM	118 CG ARG 831	29.808 50.050 21.092 1.00 12.65
ATOM	119 CD ARG 831	30.117 50.265 22.554 1.00 12.46
ATOM	120 NE ARG 831	31.261 51.148 22.584 1.00 20.55
ATOM	122 CZ ARG 831	32.469 50.756 22.885 1.00 12.04
ATOM	123 NH1 ARG 831	32.688 49.518 23.234 1.00 23.80
ATOM	126 NH2 ARG 831	33.467 51.501 22.526 1.00 23.84
ATOM	129 C ARG 831	26.625 50.415 19.174 1.00 18.55
ATOM	130 O ARG 831	25.852 49.561 19.607 1.00 25.61
ATOM	131 N ASP 832	26.221 51.517 18.552 1.00 25.32
ATOM	133 CA ASP 832	24.794 51.734 18.354 1.00 29.47
ATOM	134 CB ASP 832	24.393 53.230 18.408 1.00 34.15
ATOM	135 CG ASP 832	24.817 54.036 17.174 1.00 33.50
ATOM	136 OD1 ASP 832	25.519 53.528 16.280 1.00 34.09
ATOM	137 OD2 ASP 832	24.422 55.216 17.110 1.00 41.48
ATOM	138 C ASP 832	24.230 51.000 17.139 1.00 27.13
ATOM	139 O ASP 832	23.023 50.905 16.991 1.00 28.08
ATOM	140 N ARG 833	25.104 50.466 16.290 1.00 24.18
ATOM	142 CA ARG 833	24.684 49.695 15.134 1.00 19.93
ATOM	143 CB ARG 833	25.661 49.902 14.011 1.00 25.94
ATOM	144 CG ARG 833	25.313 51.073 13.158 1.00 38.97
ATOM	145 CD ARG 833	25.929 50.901 11.766 1.00 53.19
ATOM.	146 NE ARG 833	25.525 51.930 10.807 1.00 63.47
ATOM	148 CZ ARG 833	25.419 53.229 11.087 1.00 70.42
ATOM	149 NH1 ARG 833	25.040 54.080 10.139 1.00 74.08
ATOM	152 NH2 ARG 833	25.695 53.690 12.306 1.00 72.08
ATOM	155 C ARG 833	24.656 48.218 15.498 1.00 18.62

#### FIG. 7(4)

FIG. 7(4)

ATOM 156 O ARG 833

ATOM 157 N LEU 834

ATOM 159 CA LEU 834

ATOM 160 CB LEU 834

ATOM 161 CG LEU 834

ATOM 162 CD1 LEU 834

ATOM 163 CD2 LEU 834

ATOM 163 CD2 LEU 834

ATOM 166 N LYS 835

ATOM 166 N LYS 835

ATOM 168 CA LYS 835

ATOM 170 CG LYS 835

ATOM 171 CD LYS 835

ATOM 173 NZ LYS 835

ATOM 178 O LYS 835

ATOM 178 O LYS 835

ATOM 179 N LEU 836

ATOM 181 CA LEU 836

ATOM 182 CB LEU 836

ATOM 183 CG LEU 836

ATOM 184 CD1 LEU 836

ATOM 185 CD2 LEU 836

ATOM 186 C LEU 836

ATOM 187 O LEU 836

ATOM 188 N GLY 837

ATOM 186 C LEU 836

ATOM 187 O LEU 836

ATOM 187 O LEU 836

ATOM 190 CA GLY 837

ATOM 191 C GLY 837

ATOM 191 C GLY 837

ATOM 183 NG LYS 835

ATOM 184 CD1 LEU 836

ATOM 185 CD2 LEU 836

ATOM 187 O LEU 836

ATOM 187 O LEU 836

ATOM 191 C GLY 837

ATOM 192 C GLY 837

ATOM 195 CA LYS 835

ATOM 197 C LYS 838

ATOM 197 C LYS 838

ATOM 197 C LYS 838

ATOM 197 C LYS 837

ATOM 198 O LEU 836

ATOM 199 CA GLY 837

ATOM 190 CA GLY 837

ATOM 191 C GLY 837

ATOM 192 O GLY 837

ATOM 193 N LYS 838

ATOM 194 C BLYS 838

ATOM 195 CA LYS 838

ATOM 196 CB LYS 838

ATOM 197 C LYS 838

ATOM 198 O PRO 839

ATOM 199 O A GLY 837

ATOM 190 CA GLY 837

ATOM 190 CA GLY 837

ATOM 191 C GLY 837

ATOM 191 C GLY 837

ATOM 192 O GLY 837

ATOM 193 N LYS 838

ATOM 196 CB LYS 838

ATOM 197 C LYS 838

ATOM 197 C LYS 838

ATOM 198 O PRO 839

ATOM 200 CD PRO 839

ATOM 201 CA PRO 839

ATOM 204 C PRO 839

ATOM 205 O PRO 839

ATOM 205 O PRO 839

ATOM 206 N LEU 840

24.289 47.370 14.6490 1.00 12.329

24.289 47.370 14.6600 1.7329 1.00 24.64

25.084 44.327 16.805 1.00 17.43

25.084 46.329 17.946 1.00 25.91

24.289 24.269 18.616 1.00 34.57

ATOM 199 N PRO 839

ATOM 206 CD PRO 839

ATOM 207 CD PRO 839

ATOM 208 O PRO 839

ATOM 209 CD PRO 839

ATOM 206 O PRO 839

ATOM 207 CPRO 839

ATOM 208 CPRO 839

ATOM 208 CPRO 839

ATOM 208 CPRO 839

ATOM 206 O PRO 839

AT

#### FIG. 7(5)

ATOM 208 CA LEU 840 26.646 31.915 21.917 1.00 47.73 ATOM 209 CB LEU 840 27,396 32,426 20,692 1,00 41,83 ATOM 210 CG LEU 840 26.386 32.957 19.697 1.00 39.60 ATOM 211 CD1 LEU 840 27,080 33.697 18.595 1.00 42.69 25.582 31.795 19.156 1.00 38.40 ATOM 212 CD2 LEU 840 27.523 30.987 22.747 1.00 54.84 ATOM 213 C LEU 840 27.479 29.768 22.577 1.00 59.76 ATOM 214 O LEU 840 ATOM 215 N GLY 841 28,248 31,563 23,706 1,00 60,51 ATOM 217 CA GLY 841 29,140 30,781 24,547 1,00 60,96 ATOM 218 C GLY 841 29,660 31,544 25,750 1,00 63,95 30.279 30.809 26.668 1.00 65.26 30.823 31.388 27 997 100 29,497 32,764 25,857 1.00 64,35 ATOM 219 O GLY 841 ATOM 220 N ARG 842 ATOM 222 CA ARG 842 ATOM 223 CB ARG 842 30.027 30.897 29.091 1.00 61.50 ATOM 224 C ARG 842 32,300 30,995 28,004 1,00 64,23 ATOM 225 O ARG 842 32,957 30,720 26,986 1,00 68,80 32.822 31.003 29.226 1.00 60.14 ATOM 226 N GLY 843 34,206 30,639 29,453 1.00 60,53 ATOM 228 CA GLY 843 34.676 31.165 30.789 1.00 62.56 ATOM 229 C GLY 843 ATOM 230 O GLY 843 33,902 31.764 31.535 1.00 61.31 ATOM 231 N ALA 844 35,925 30.888 31.140 1.00 66.30 36.450 31.390 32.403 1.00 69.69 37.655 30.574 32.851 1.00 68.47 ATOM 233 CA ALA 844 ATOM 234 CB ALA 844 ATOM 235 C ALA 844 36,839 32,855 32,212 1.00 73,15 36.723 33.667 33.144 1.00 75.00 ATOM 236 O ALA 844 37.251 33.184 30.981 1.00 76.12 ATOM 237 N PHE 845 ATOM 239 CA PHE 845 37,699 34,538 30,618 1,00 74,99 ATOM 240 CB PHE 845 39.135 34.479 30.014 1.00 72.01 ATOM 241 C PHE 845 36,766 35,353 29,700 1.00 73.81 ATOM 242 O PHE 845 36,404 36,499 30,020 1,00 76,82 ATOM 243 N GLY 846 36.368 34.767 28.576 1.00 68.48 ATOM 245 CA GLY 846 35.527 35.495 27.645 1.00 61.76 ATOM 246 C GLY 846 34.102 35.023 27.606 1.00 57.98 ATOM 247 O GLY 846 33,658 34,305 28,491 1,00 59,43 ATOM 248 N GLN 847 33,400 35,413 26,553 1.00 55.08 32,006 35,050 26,354 1,00 52,26 ATOM 250 CA GLN 847 ATOM 251 CB GLN 847 31,160 35,668 27,449 1,00 55,14 ATOM 252 CG GLN 847 29,706 35,703 27,075 1,00 61,40 ATOM 253 CD GLN 847 28,951~36,735 27,844 1,00 65,75 ATOM 254 OE1 GLN 847 27.772 36.543 28.150 1.00 69.74 29.614 37.852 28.166 1.00 68.83 ATOM 255 NE2 GLN 847 31,508 35,573 25,001 1,00 47,29 ATOM 258 C GLN 847 ATOM 259 O GLN 847 31.637 36.764 24.713 1.00 52.89

#### FIG. 7(6)

30.912 34.707 24.195 1.00 38.17 ATOM 260 N VAL 848 30.512 54.707 24.195 1.00 53.028 30.792 34.137 21.833 1.00 28.01 30.542 34.744 20.442 1.00 23.32 32.239 33.759 22.016 1.00 22.18 28.920 35.262 22.939 1.00 31.80 ATOM 262 CA VAL 848 ATOM 263 CB VAL 848 ATOM 264 CG1 VAL 848 ATOM 265 CG2 VAL 848 ATOM 266 C VAL 848 28,221 34,525 23,625 1.00 32.87 ATOM 267 O VAL 848 28,221 34,525 23,625 1.00 32.87 ATOM 270 CA ILE 849 26,699 36,436 22,159 1.00 25,35 ATOM 271 CB ILE 849 26,602 37,448 23,328 1.00 31.46 ATOM 273 CG1 ILE 849 27,766 38,373 23,732 1.00 31.00 ATOM 274 CD1 ILE 849 25,353 38,244 23,003 1.00 31.00 ATOM 274 CD1 ILE 849 26,493 36,851 20,798 1.00 23,02 ATOM 276 O ILE 849 27,167 37,540 20,070 1.00 27,56 ATOM 279 CA GLU 850 25,376 36,294 20,390 1.00 25,56 ATOM 279 CA GLU 850 24,802 36,626 19,107 1.00 26,63 ATOM 280 CB GLU 850 23,577 35,785 18,894 1.00 27,45 ATOM 281 CG GLU 850 23,414 35,361 17,487 1.00 34,46 ATOM 267 O VAL 848 ATOM 280 CB GLU 850 ATOM 281 CG GLU 850 ATOM 282 CD GLU 850 ATOM 281 CG GLU 850
ATOM 282 CD GLU 850
ATOM 283 OEI GLU 850
ATOM 284 OE2 GLU 850
ATOM 285 C GLU 850
ATOM 286 OELU 850
ATOM 286 O GLU 850
ATOM 286 O GLU 850
ATOM 287 N ALA 851
ATOM 289 CA ALA 851
ATOM 290 CB ALA 851
ATOM 291 C ALA 851
ATOM 292 O ALA 851
ATOM 292 O ALA 851
ATOM 293 N ASP 852
ATOM 295 CA ASP 852
ATOM 296 CB ASP 852
ATOM 297 CG ASP 852
ATOM 298 ODI ASP 852
ATOM 298 ODI ASP 852
ATOM 299 OD2 ASP 852
ATOM 290 C ASP 852
ATOM 290 CA SP 852
ATOM 291 CA SP 852
ATOM 295 CA ASP 852
ATOM 296 CB ASP 852
ATOM 297 CG ASP 852
ATOM 298 ODI ASP 852
ATOM 300 C ASP 852
ATOM 300 C ASP 852
ATOM 301 O ASP 852
ATOM 302 N ALA 853
ATOM 305 CB ALA 853
ATOM 305 CB ALA 853
ATOM 307 O ALA 853
ATOM 308 N PHE 854

23.414 35.501 17.023 1.00 34.46
24.422 38.111 19.028 1.00 27.83
24.242 38.131 1 19.028 1.00 29.18
24.242 38.755 20.047 1.00 29.11
24.242 38.755 20.047 1.00 29.11
24.242 38.755 20.047 1.00 29.11
24.240 38.755 20.047 1.00 29.11
24.240 38.755 20.047 1.00 29.11
24.240 38.755 20.047 1.00 29.11
24.240 38.755 20.047 1.00 29.11
24.240 38.755 20.047 1.00 29.11
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.240 38.755 20.047 1.00 29.18
24.311 45.222 12.026 1.00 23.39
24.044 46.526 11.936 1.00 22.87

#### FIG. 7(7)

ATOM 310 CA PHE 854 23.529 47.059 10.680 1.00 16.46 22.487 48.135 10.901 1.00 23.71 22.020 48.758 9.643 1.00 27.62 22.476 50.011 9.266 1.00 28.26 21.205 48.052 8.771 1.00 31.56 22.136 50.549 8.025 1.00 30.16 20.856 48.592 7.512 1.00 34.04 21.328 49.838 7.145 1.00 28.32 24.618 47.569 9.794 1.00 14.10 25.493 48.299 10.209 1.00 17.34 24.556 47 163 8553 1.00 17.45 22,487 48,135 10,901 1,00 23,71 ATOM 311 CB PHE 854 ATOM 312 CG PHE 854 ATOM 313 CD1 PHE 854 ATOM 314 CD2 PHE 854 ATOM 315 CE1 PHE 854 ATOM 316 CE2 PHE 854 ATOM 317 CZ PHE 854 ATOM 318 C PHE 854 25.493 48.299 10.209 1.00 17.34
24.556 47.163 8.553 1.00 17.45
25.559 47.571 7.604 1.00 18.50
26.988 47.318 8.020 1.00 22.65
27.806 48.193 7.777 1.00 26.82
27.332 46.150 8.580 1.00 23.51
28.740 45.886 8.983 1.00 24.11
28.868 44.692 9.980 1.00 27.72
28.555 43.370 9.259 1.00 29.88
30.282 44.663 10.608 1.00 23.26
30.371 44.079 12.034 1.00 21.70
29.704 45.665 7.805 1.00 24.83
30.918 45.721 7.950 1.00 28.37
29.145 45.460 6.626 1.00 27.69
29.926 45.248 5.420 1.00 31.23
29.566 43.891 4.838 1.00 34.80
28.074 43.658 4.811 1.00 40.03 ATOM 319 O PHE 854 ATOM 319 O PHE 854
ATOM 320 N GLY 855
ATOM 322 CA GLY 855
ATOM 323 C GLY 855
ATOM 324 O GLY 855
ATOM 325 N ILE 856
ATOM 327 CA ILE 856
ATOM 328 CB ILE 856
ATOM 329 CG2 ILE 856
ATOM 330 CG1 ILE 856
ATOM 331 CD1 ILE 856
ATOM 332 C ILE 856
ATOM 333 O ILE 856
ATOM 333 O ILE 856
ATOM 334 N ASP 857 ATOM 334 N ASP 857 ATOM 336 CA ASP 857 29.566 43.891 4.830 1.00 40.03 28.074 43.658 4.811 1.00 40.03 27.328 44.597 4.448 1.00 43.33 27.541 42.549 5.200 1.00 46.87 ATOM 337 CB ASP 857 ATOM 338 CG ASP 857 ATOM 330 OD1 ASP 857 ATOM 340 OD2 ASP 857 ATOM 341 C ASP 857 ATOM 342 O ASP 857 ATOM 343 N LYS 858 ATOM 345 CA LYS 858 29.654 46.323 4.370 1.00 32.81 29.721 46.040 3.183 1.00 38.59 29.299 47.529 4.813 1.00 34.74 28.987 48.690 3.946 1.00 34.64 30.061 48.947 2.889 1.00 31.38 31.462 48.964 3.418 1.00 34.36 ATOM 346 CB LYS 858 ATOM 347 CG LYS 858 31.605 49.890 4.603 1.00 39.41 ATOM 348 CD LYS 858 ATOM 349 CE LYS 858 33.005 49.791 5.228 1.00 39.87 34.059 50.089 4.218 1.00 39.89 27.629 48.709 3.254 1.00 32.27 33.005 49.791 5.228 1.00 39.87 ATOM 350 NZ LYS 858 ATOM 354 C LYS 858 ATOM 355 O LYS 858 27,249 49,737 2,724 1,00 35,02 ATOM 355 O LYS 858 27.249 49.737 2.724 1.00 35.02 ATOM 356 N THR 859 26.891 47.607 3.258 1.00 32.20 ATOM 359 CB THR 859 25.597 47.610 2.600 1.00 30.11 ATOM 360 OG1 THR 859 25.365 45.187 2.641 1.00 32.29 ATOM 359 CB THR 859 ATOM 360 OG1 THR 859

#### FIG. 7(8)

ATOM 362 CG2 THR 859 26.437 46.179 0.757 1.00 32.22 4.450 47.839 3.546 1.00 28.71 ATOM 364 O THR 859 24.577 47.647 4.750 1.00 30.55 ATOM 365 N ALA 860 23.303 48.201 2.989 1.00 30.07 ATOM 367 CA ALA 860 21.141 49.253 2.928 1.00 23.78 ATOM 369 C ALA 860 21.141 49.253 2.928 1.00 23.78 ATOM 370 O ALA 860 20.251 47.100 4.373 1.00 31.77 ATOM 371 N THR 861 22.284 46.325 5.008 1.00 29.99 ATOM 373 CA THR 861 21.663 45.078 5.577 1.00 27.77 ATOM 377 CG2 THR 861 23.614 43.926 4.687 1.00 27.23 ATOM 378 C THR 861 21.698 43.794 3.449 1.00 29.39 ATOM 378 C THR 861 21.986 44.790 7.055 1.00 31.89 ATOM 362 CG2 THR 859 26,437 46,179 0,757 1,00 32,22 ATOM 375 OG1 THR 861 ATOM 377 CG2 THR 861 ATOM 378 C THR 861 21,986 44,790 7.055 1.00 31.89 ATOM 379 O THR 861 23,095 45.077 7.532 1.00 34.73 ATOM 380 N CYS 862 21,037 44,183 7.770 1.00 34.09 ATOM 382 CA CYS 862 21,250 43,805 9,178 1.00 34.63 ATOM 383 CB CYS 862 19,922 43,756 9,943 1.00 27.50 ATOM 384 SG CYS 862 19,863 44,908 11,327 1.00 41,79 ATOM 385 C CYS 862 21.876 42.424 9.146 1.00 25.51 ATOM 386 C CYS 862 21.24 41.492 8.700 1.00 25.35 ATOM 387 N ARG 863 23.136 42.307 9.541 1.00 27.68 ATOM 389 CA ARG 863 23.839 41.025 9.532 1.00 28.29 ATOM 391 CG ARG 863 25.211 41.210 8.882 1.00 36.18 ATOM 392 CD ARG 863 25.275 39.945 8.275 1.00 48.71 ATOM 393 NE ARG 863 27.824 40.034 7.943 1.00 58.46 ATOM 393 NE ARG 863 27.824 38.721 7.550 1.00 65.04 ATOM 395 CZ ADC 863 27.824 38.721 7.550 1.00 65.04 ATOM 386 O CYS 862 27.024 56.721 7.530 1.00 05.04 29.112 38.452 7.330 1.00 65.66 29.482 37.219 6.985 1.00 67.60 30.030 39.409 7.421 1.00 66.49 24.006 40.409 10.943 1.00 28.34 24.337 41.125 11.904 1.00 24.64 23.735 39.100 11.078 1.00 23.23 23.900 38.426 12.364 1.00 18.91 ATOM 395 CZ ARG 863 ATOM 396 NH1 ARG 863 ATOM 399 NH2 ARG 863 ATOM 402 C ARG 863 ATOM 403 O ARG 863 ATOM 404 N THR 864 ATOM 406 CA THR 864 ATOM 407 CB THR 864 23.062 37.099 12.489 1.00 19.40 ATOM 408 OG1 THR 864 23.062 37.099 12.489 1.00 19.40
ATOM 410 CG2 THR 864 21.672 37.435 12.547 1.00 24.20
ATOM 411 C THR 864 23.371 36.351 13.793 1.00 8.83
ATOM 412 O THR 864 25.385 38.148 12.462 1.00 20.93
ATOM 413 N VAL 865 25.962 38.442 13.634 1.00 16.03
ATOM 415 CA VAL 865 27.381 38.254 13.897 1.00 16.69
ATOM 416 CB VAL 865 28.175 39.620 13.906 1.00 17.70
ATOM 417 CG1 VAL 865 28.107 40.299 12.539 1.00 21.22

#### FIG. 7(9)

ATOM 418 CG2 VAL 865 27,625 40,554 14,979 1,00 20,92 27.533 37.660 15.276 1.00 15.90 ATOM 419 C VAL 865 ATOM 420 O VAL 865 26.552 37.554 15.995 1.00 16.43 ATOM 421 N ALA 866 28,775 37,295 15.612 1.00 16.37 28.775 37.295 15.612 1.00 16.37 29.210 36.753 16.910 1.00 18.08 30.022 35.490 16.691 1.00 7.41 ATOM 423 CA ALA 866 ATOM 424 CB ALA 866 ATOM 425 C ALA 866 30.117 37.834 17.588 1.00 23.87 ATOM 426 O ALA 866 31.121 38.261 16.998 1.00 24.17 31.121 38.261 16.998 1.00 24.17 29.790 38.235 18.827 1.00 26.69 427 N VAL 867 ATOM ATOM 429 CA VAL 867 30.534 39.268 19.554 1.00 20.37 29,592 40,365 20,088 1.00 17.71 430 CB VAL 867 ATOM 30.361 41.586 20.519 1.00 9.32 28.635 40.753 19.027 1.00 14.57 431 CG1 VAL 867 ATOM 432 CG2 VAL 867 ATOM 433 C VAL 867 31.320 38.748 20.728 1.00 21.67 ATOM 30.784 38.085 21.606 1.00 23.57 32.616 38.982 20.694 1.00 21.65 ATOM 434 O VAL 867 435 N LYS 868 ATOM 33,471 38,593 21,782 1.00 27.02 ATOM 437 CA LYS 868 34.860 38.169 21.289 1.00 29.71 ATOM 438 CB LYS 868 34.842 36.963 20.405 1.00 37.08 ATOM 439 CG LYS 868 36.151 36.810 19.666 1.00 44.81 ATOM 440 CD LYS 868 36.183 35.512 18.868 1.00 45.52 ATOM 441 CE LYS 868 ATOM 442 NZ LYS 868 37.548 35.298 18.274 1.00 47.28 33.585 39.842 22.647 1.00 26.11 ATOM 446 C LYS 868 ATOM 447 O LYS 868 33,962 40,914 22,188 1,00 24,72 33.184 39.721 23.888 1.00 29.77 33.299 40.821 24.803 1.00 32.95 31.958 41.491 24.996 1.00 30.57 448 N MET 869 ATOM ATOM 450 CA MET 869 ATOM 451 CB MET 869 ATOM 452 CG MET 869 30,900 40,542 25,463 1,00 32,29 ATOM 453 SD MET 869 29.348 41.157 24.961 1.00 42.68 29,348 41.157 24.961 1.00 42.68 29,251 42.663 25.919 1.00 35.32 33,778 40.205 26.095 1.00 40.29 33,921 38.967 26.216 1.00 35.26 34,079 41.066 27.051 1.00 46.88 ATOM 454 CE MET 869 ATOM 455 C MET 869 ATOM 456 O MET 869 ATOM 457 N LEU 870 ATOM 459 CA LEU 870 34,521 40,576 28,337 1.00 51.36 ATOM 460 CB LEU 870 35.544 41.549 28.937 1.00 48.55 36.862 41.677 28.180 1.00 44.32 ATOM 461 CG LEU 870 37.734 42.739 28.855 1.00 36.89 ATOM 462 CD1 LEU 870 37.535 40.306 28.149 1.00 41.04 ATOM 463 CD2 LEU 870 33,344 40,306 29,311 1.00 53,63 32,163 40,615 29,037 1.00 52,68 464 C LEU 870 ATOM ATOM 465 O LEU 870 33.675 39.644 30.412 1.00 56.89 466 N LYS 871 ATOM 32.695 39.346 31.426 1.00 58.53 ATOM 468 CA LYS 871 33,083 38,077 32,169 1,00 59,89 469 CB LYS 871 ATOM

#### FIG. 7(10)

ATOM 470 CG LYS 871 31,903 37,220 32,546 1.00 63.81 31.912 35.965 31.719 1.00 65.43
33.268 35.318 31.853 1.00 70.59
33.318 34.051 31.135 1.00 76.57
32.649 40.518 32.404 1.00 56.75
31.566 40.571 33.177 1.00 61.50
2 31.357 41.618 34.177 1.00 61.50
2 29.928 41.539 34.739 1.00 66.85
2 28.846 41.903 33.729 1.00 71.27
2 90.60 41.218 32.387 1.00 74.41
2 28.900 39.980 32.326 1.00 74.41
2 28.900 39.980 32.326 1.00 76.27
2 29.443 41.903 31.411 1.00 74.20
32.387 41.424 35.288 1.00 60.87
32.331 40.441 36.026 1.00 61.34
33.368 42.319 35.335 1.00 57.40
3 34.408 42.223 36.337 1.00 53.93 ATOM 471 CD LYS 871 31,912 35,965 31,719 1.00 65,43 ATOM 472 CE LYS 871 ATOM 473 NZ LYS 871 ATOM 477 C LYS 871 ATOM 478 O LYS 871 ATOM 479 N GLU 872 ATOM 481 CA GLU 872 ATOM 482 CB GLU 872 ATOM 482 CB GLU 872
ATOM 483 CG GLU 872
ATOM 484 CD GLU 872
ATOM 485 OE1 GLU 872
ATOM 486 OE2 GLU 872
ATOM 487 C GLU 872
ATOM 488 O GLU 872
ATOM 489 N GLY 873
ATOM 491 CA GLY 873
ATOM 492 C GLY 873
ATOM 493 O GLY 873
ATOM 494 N ALA 874
ATOM 496 CA ALA 874
ATOM 497 CB ALA 874
ATOM 498 C ALA 874 34.408 42.223 36.337 1.00 53.93 ATOM 491 CA GLY 873
ATOM 492 C GLY 873
ATOM 493 O GLY 873
ATOM 494 N ALA 874
ATOM 496 CA ALA 874
ATOM 497 CB ALA 874
ATOM 498 C ALA 874
ATOM 499 O ALA 874
ATOM 500 N THR 875
ATOM 502 CA THR 875
ATOM 504 CGL THR 875 ATOM 503 CB THR 875 42.677 42.184 35.937 1.00 60.69 42.107 40.280 34.593 1.00 60.52 41.455 42.830 33.448 1.00 51.15 41.395 42.263 32.372 1.00 52.26 ATOM 504 OG1 THR 875 ATOM 506 CG2 THR 875 ATOM 507 C THR 875 ATOM 508 O THR 875
ATOM 509 N HIS 876
ATOM 511 CA HIS 876
ATOM 512 CB HIS 876
ATOM 512 CB HIS 876
ATOM 514 CD2 HIS 876
ATOM 515 ND1 HIS 876
ATOM 515 ND1 HIS 876
ATOM 517 CE1 HIS 876
ATOM 517 CE1 HIS 876
ATOM 518 NE2 HIS 876
ATOM 520 C HIS 876
ATOM 521 O HIS 876
ATOM 520 C HIS 876
ATOM 521 O HIS 876
ATOM 520 C HIS 876
ATOM 521 O HIS 876
ATOM 520 C HIS 876
ATOM 521 O HIS 876
ATOM 521 O HIS 876
ATOM 521 O HIS 876
ATOM 522 N SER 877
ATOM 524 CA SER 877
ATOM 524 CA SER 877 ATOM 508 O THR 875 . ATOM 513 CG HIS 876 ATOM 524 CA SER 877

#### FIG. 7(11)

ATOM 525 CB SER 877
ATOM 526 OG SER 877
ATOM 528 C SER 877
ATOM 529 O SER 877
ATOM 529 O SER 877
ATOM 530 N GLU 878
ATOM 531 CB GLU 878
ATOM 532 CB GLU 878
ATOM 535 CB GLU 878
ATOM 535 CB GLU 878
ATOM 536 OEI GLU 878
ATOM 537 OE2 GLU 878
ATOM 539 O GLU 878
ATOM 539 C GLU 878
ATOM 539 C GLU 878
ATOM 530 R GLU 878
ATOM 534 CG GLU 878
ATOM 536 OEI GLU 878
ATOM 537 OE2 GLU 878
ATOM 537 OE2 GLU 878
ATOM 539 C GLU 878
ATOM 530 R GLU 878
ATOM 539 C GLU 878
ATOM 539 C GLU 878
ATOM 539 C GLU 878
ATOM 540 CR HIS 879
ATOM 540 CR HIS 879
ATOM 540 CR HIS 879
ATOM 544 CG HIS 879
ATOM 545 CDZ HIS 879
ATOM 546 NDI HIS 879
ATOM 547 CH HIS 879
ATOM 548 CE HIS 879
ATOM 549 NE2 HIS 879
ATOM 557 CA ARG 880
ATOM 557 CA ARG 880
ATOM 557 CG ARG 880
ATOM 558 C ARG 880
ATOM 558 C ARG 880
ATOM 558 C ARG 880
ATOM 559 NE ARG 880
ATOM 557 CG ARG 880
ATOM 557 CG ARG 880
ATOM 558 C ARG 880
ATOM 558 C ARG 880
ATOM 559 NE ARG 880
ATOM 557 O ALA 881
ATOM 570 C ALA 881
ATOM 570 C ALA 881
ATOM 575 O ALA 881
ATOM 575 O ALA 881
ATOM 575 O BLEU 882
ATOM 579 CB LEU 882
ATOM 579 CB LEU 882
ATOM 580 CG LEU 882
39.493 40.784 24.728 1.00 23.93

#### FIG. 7(12)

ATOM 581 CD1 LEU 882 38.435 39.722 22.743 1.00 21.91 ATOM 582 CD2 LEU 882 37,013 41,102 24,325 1,00 23,61 ATOM 583 C LEU 882 41,368 41,230 23,151 1.00 30,62 41.312 40.982 21.945 1.00 27.61 ATOM 584 O LEU 882 ATOM 585 N MET 883 41.940 42.325 23.643 1.00 29.74 ATOM 587 CA MET 883 42,548 43,364 22,808 1,00 30,75 43.001 44.516 23.738 1.00 27.47 43.432 45.828 23.084 1.00 33.64 ATOM 588 CB MET 883 ATOM 589 CG MET 883 ATOM 590 SD MET 883 42.313 46.592 21.882 1.00 33.18 41.031 47.285 22.943 1.00 33.54 ATOM 591 CE MET 883 43.711 42.756 21.965 1.00 29.92 ATOM 592 C MET 883 ATOM 592 C MET 883
ATOM 593 O MET 883
ATOM 594 N SER 884
ATOM 596 CA SER 884
ATOM 597 CB SER 884
ATOM 600 C SER 884
ATOM 601 O SER 884
ATOM 602 N GLU 885
ATOM 606 CG GLU 885
ATOM 606 CG GLU 885
ATOM 607 CD GLU 885
ATOM 607 CD GLU 885
ATOM 608 OFI GLU 885 43,862 43,022 20,766 1.00 28,38 44.501 41.893 22.586 k.00 2 45.597 41.231 21.912 1.00 28.29 46.343 40.391 22.923 1.00 32.03 45.091 40.329 20.778 1.00 29.39 45.595 40.359 19.654 1.00 28.92 44,084 39,526 21,071 1,00 25,33 43.559 38.661 20.058 1.00 27.47 42.563 37.692 20.661 1.00 31.61 41.142 38.108 20.642 1.00 46.01 40.215 36.903 20.799 1.00 55.19 40.018 36.469 21.964 1.00 58.80 39.715 36.379 19.762 1.00 54.01 ATOM 608 OE1 GLU 885 ATOM 609 OE2 GLU 885 42.945 39.470 18.924 1.00 28.59 ATOM 610 C GLU 885 42,833 38,983 17,805 1,00 26,67 ATOM 611 O GLU 885 ATOM 612 N LEU 886 42.560 40.712 19.211 1.00 27.06 ATOM 614 CA LEU 886 ATOM 615 CB LEU 886 ATOM 616 CG LEU 886 41.994 41.594 18.205 1.00 23.75 41,483 42,887 18,847 1,00 22,79 41.122 44.033 17.905 1.00 17.60 39.981 43.609 16.000 1.00 1.00 39.981 43.608 16.999 1.00 11.98 ATOM 617 CD1 LEU 886 ATOM 618 CD2 LEU 886 40,747 45,285 18,702 1,00 18,31 ATOM 619 C LEU 886 43.049 41.936 17.147 1.00 24.77 42.767 41.880 15.939 1.00 22.15 ATOM 620 O LEU 886 ATOM 621 N LYS 887 44.265 42.246 17.602 1.00 25.08 ATOM 623 CA LYS 887 45,384 42,613 16,722 1,00 24,94 46.517 43.227 17.544 1.00 29.70 46.105 44.304 18.560 1.00 30.67 ATOM 624 CB LYS 887 ATOM 625 CG LYS 887 45.556 45.551 17.895 1.00 28.99 ATOM 626 CD LYS 887 ATOM 626 CD LYS 887 45.550 45.551 17.695 1.00 26.77 ATOM 627 CE LYS 887 45.170 46.645 18.923 1.00 26.07 ATOM 628 NZ LYS 887 46.354 47.216 19.621 1.00 17.59 ATOM 632 C LYS 887 45,921 41,407 15,925 1,00 25,59

#### FIG. 7(13)

FIG. 7(13)

ATOM 633 O LYS 887
ATOM 634 N ILE 888
ATOM 636 CA ILE 888
ATOM 637 CB ILE 888
ATOM 638 CG2 ILE 888
ATOM 639 CG1 ILE 888
ATOM 640 CD1 ILE 888
ATOM 641 C ILE 888
ATOM 642 O ILE 888
ATOM 645 CA LEU 889
ATOM 646 CB LEU 889
ATOM 646 CB LEU 889
ATOM 647 CG LEU 889
ATOM 648 CD1 LEU 889
ATOM 649 CD2 LEU 889
ATOM 650 C LEU 889
ATOM 650 C LEU 889
ATOM 651 O LEU 889
ATOM 651 O LEU 889
ATOM 650 C LEU 889
ATOM 651 O LEU 889
ATOM 650 C LEU 889
ATOM 650 C LEU 889
ATOM 651 O LEU 889
ATOM 650 C LEU 890
ATOM 650 C LEU 800
ATO ATOM 672 C HIS 891 47.098 39.536 10.537 1.00 27.01
ATOM 673 O HIS 891 47.522 39.647 9.402 1.00 32.82
ATOM 674 N ILE 892 46.580 38.403 10.995 1.00 24.99
ATOM 676 CA ILE 892 46.300 37.216 10.181 1.00 23.19
ATOM 677 CB ILE 892 45.233 36.282 10.907 1.00 24.73
ATOM 679 CG1 ILE 892 44.643 35.295 9.941 1.00 20.03
ATOM 680 CD1 ILE 892 45.828 35.522 12.104 1.00 26.32
ATOM 681 C ILE 892 45.700 37.625 8.848 1.00 22.57
ATOM 682 O ILE 892 46.115 37.155 7.775 1.00 25.20

## FIG. 7(14)

ATOM	683 N GLY 893	44.699 38.492	8.916 1.00 23.88
ATOM	685 CA GLY 893	44.034 38.910	7.702 1.00 25.37
ATOM	686 C GLY 893	42.794 38.080	7.403 1.00 25.54
ATOM	687 O GLY 893	42.303 37.326	8.224 1.00 32.60
ATOM	688 N HIS 894	42.327 38.149	6.176 1.00 26.97
ATOM	690 CA HIS 894	41.120 37.457	5.797 1.00 26.35
ATOM	691 CB HIS 894	40.233 38.464	5.042 1.00 31.72
ATOM	692 CG HIS 894	39.114 37.833	4.274 1.00 35.68
ATOM	693 CD2 HIS 894	37.818 37.609	4.608 1.00 34.18
ATOM	694 ND1 HIS 894	39.271 37.346	2.989 1.00 38.36
ATOM	696 CE1 HIS 894	38.121 36.854	2.568 1.00 36.24
ATOM	697 NE2 HIS 894	37.224 37.004	3.527 1.00 35.86
ATOM	699 C HIS 894	41.253 36.182	4.958 1.00 24.38
ATOM	700 O HIS 894	42.045 36.108	4.007 1.00 24.24
ATOM	701 N HIS 895	40.426 35.202	5.280 1.00 17.00
ATOM	703 CA HIS 895	40.379 33.994	4.494 1.00 18.62
ATOM	704 CB HIS 895	41.363 32.929	4.931 1.00 15.85
ATOM	705 CG HIS 895	41.446 31.814	3.943 1.00 21.47
ATOM	706 CD2 HIS 895	42.076 31.737	2.745 1.00 17.93
ATOM	707 ND1 HIS 895	40.675 30.676	4.042 1.00 21.96
ATOM	709 CE1 HIS 895	40.819 29.956	2.938 1.00 21.22
ATOM	710 NE2 HIS 895	41.663 30.578	2.137 1.00 10.16
ATOM	712 C HIS 895	38.979 33.467	4.626 1.00 15.66
ATOM	713 O HIS 895	38.396 33.656	5.663 1.00 18.76
ATOM	714 N LEU 896	38.419 32.865	3.567 1.00 21.74
ATOM	716 CA LEU 896	37.042 32.306	3.584 1.00 18.37
ATOM	717 CB LEU 896	36.652 31.762	2.210 1.00 17.64
ATOM	718 CG LEU 896	35.297 31.068	2.218 1.00 25.15
ATOM	719 CD1 LEU 896	34.218 32.077	2.454 1.00 24.41
ATOM	720 CD2 LEU 896	35.042 30.342	0.934 1.00 25.59
ATOM	721 C LEU 896	36.867 31.172	4.569 1.00 17.58
ATOM	722 O LEU 896	35.783 30.937	5.068 1.00 23.11
ATOM	723 N ASN 897	37.952 30.475	4.849 1.00 15.99
ATOM	725 CA ASN 897	37.878 29.340	5.725 1.00 18.36
ATOM	726 CB ASN 897	38.589 28.134	5.078 1.00 20.86
ATOM	727 CG ASN 897	37.928 27.689	3.747 1.00 16.88
ATOM	728 OD1 ASN 897	38.567 27.692	2.694 1.00 14.51
ATOM	729 ND2 ASN 897	36.639 27.346	3.799 1.00 12.11
ATOM	732 C ASN 897	38.293 29.541	7.188 1.00 25.65
ATOM	733 O ASN 897	38.648 28.556	7.858 1.00 22.22
ATOM	734 N VAL 898	38.357 30.800	7.660 1.00 23.53
ATOM	736 CA VAL 898	38.631 31.079	9.081 1.00 15.38
ATOM	737 CB VAL 898	40.036 31.719	9.457 1.00 11.47

#### FIG. 7(15)

ATOM 738 CG1 VAL 898 41.146 30.813 9.017 1.00 14.76 ATOM 739 CG2 VAL 898 40,236 33,119 8,883 1.00 8,71 740 C VAL 898 37.475 31.959 9.477 1.00 15.57 ATOM ATOM 741 O VAL 898 36,698 32,382 8,620 1,00 17,87 ATOM 742 N VAL 899 37,226 32,049 10,773 1,00 18,55 36.155 32.882 11.264 1.00 20.68 744 CA VAL 899 ATOM ATOM 745 CB VAL 899 35.757 32.487 12.720 1.00 19.98 34.618 33.384 13.402 1.00 12.67 35.346 31.016 12.788 1.00 12.67 36.807 34.272 11.244 1.00 21.95 ATOM 746 CG1 VAL 899 ATOM 747 CG2 VAL 899 748 C VAL 899 ATOM 749 O VAL 899 ATOM 36.352 35.164 10.363 1.00 23.43 36.930 36.526 10.226 1.00 23.52 ATOM 750 N ASN 900 ATOM 752 CA ASN 900 ATOM 753 CB ASN 900 36.737 37.061 8.803 1.00 19.45 ATOM 37,350 36,177 7,782 1,00 19,58 754 CG ASN 900 38.578 36.087 7.667 1.00 17.65 36.511 35.528 7.004 1.00 20.34 ATOM 755 OD1 ASN 900 ATOM 756 ND2 ASN 900 759 C ASN 900 ATOM 36.484 37.641 11.152 1.00 17.00 ATOM 760 O ASN 900 35.343 37.704 11.598 1.00 16.94 37.413 38.544 11.384 1.00 17.25 ATOM 761 N LEU 901 ATOM 763 CA LEU 901 37.167 39.733 12.160 1.00 17.98 ATOM 764 CB LEU 901 38,494 40,447 12,426 1.00 16.80 38.444 41.819 13.101 1.00 14.17 38.018 41.673 14.560 1.00 11.71 ATOM 765 CG LEU 901 ATOM 766 CD1 LEU 901 767 CD2 LEU 901 39,782 42,435 13,008 1,00 2,76 ATOM ATOM 768 C LEU 901 36.354 40.578 11.174 1.00 20.28 36.669 40.612 9.965 1.00 18.06 ATOM 769 O LEU 901 ATOM 770 N LEU 902 35,280 41,180 11,686 1,00 19,74 34.398 42.031 10.917 1.00 15.84 32.950 41.593 11.087 1.00 11.70 ATOM 772 CA LEU 902 ATOM 773 CB LEU 902 32.615 40.230 10.473 1.00 13.49 **ATOM** 774 CG LEU 902 ATOM 775 CD1 LEU 902 31.142 39.827 10.774 1.00 13.78 776 CD2 LEU 902 32.856 40,270 8,981 1.00 12.15 ATOM 34.566 43.486 11.345 1.00 19.59 777 C LEU 902 **ATOM** ATOM 778 O LEU 902 34,466 44,380 10,510 1,00 23,95 ATOM 779 N GLY 903 34.854 43.724 12.625 1.00 20.15 35.037 45.090 13.114 1.00 21.60 35.147 45.075 14.620 1.00 24.02 781 CA GLY 903 ATOM 782 C GLY 903 ATOM 35.070 43.991 15.194 1.00 24.02 35.070 43.991 15.194 1.00 26.53 35.305 46.236 15.269 1.00 25.19 35.411 46.293 16.740 1.00 18.80 36.830 46.074 17.177 1.00 12.62 783 O GLY 903 ATOM ATOM- 784 N ALA 904 ATOM 786 CA ALA 904 ATOM 787 CB ALA 904 ATOM 788 C ALA 904 34.886 47.559 17.386 1.00 20.83

## FIG. 7(16)

ATOM	789 O ALA 904	34.789 48.616 16.765 1.00 26.12
ATOM	790 N CYS 905	34.617 47.443 18.674 1.00 21.21
ATOM	792 CA CYS 905	34.128 48.530 19.493 1.00 19.91
ATOM	793 CB CYS 905	32.804 48.160 20.115 1.00 16.08
ATOM	794 SG CYS 905	31.561 47.894 18.851 1.00 15.32
ATOM	795 C CYS 905	35.176 48.687 20.556 1.00 23.00
ATOM	796 O CYS 905	35.245 47.890 21.486 1.00 24.21
ATOM	797 N THR 906	36.042 49.674 20.361 1.00 26.02
ATOM	799 CA THR 906	37.140 49.945 21.283 1.00 29.46
ATOM	800 CB THR 906	38.514 49.768 20.574 1.00 26.67
ATOM	801 OG1 THR 906	38.635 50.739 19.526 1.00 29.06
ATOM	803 CG2 THR 906	38.648 48.363 20.001 1.00 23.13
ATOM	804 C THR 906	37.130 51.346 21.928 1.00 30.07
ATOM	805 O THR 906	37.642 51.522 23.036 1.00 29.29
ATOM	806 N LYS 907	36.582 52.332 21.228 1.00 32.81
ATOM	808 CA LYS 907	36.554 53.686 21.745 1.00 39.38
ATOM	809 CB LYS 907	35.982 54.637 20.701 1.00 41.03
ATOM	810 CG LYS 907	34.536 54.432 20.386 1.00 48.86
ATOM	811 CD LYS 907	34.071 55.528 19.427 1.00 57.25
ATOM	812 CE LYS 907	33.996 56.878 20.143 1.00 63.62
ATOM	813 NZ LYS 907	33.688 58.001 19.213 1.00 68.81
ATOM	817 C LYS 907	35.796 53.779 23.070 1.00 44.43
ATOM	818 O LYS 907	35.094 52.867 23.442 1.00 44.52
ATOM	819 N PRO 908	36.034 54.838 23.857 1.00 49.18
ATOM	820 CD PRO 908	37.147 55.794 23.712 1.00 50.93
ATOM	821 CA PRO 908	35.358 55.022 25.149 1.00 46.86
ATOM	822 CB PRO 908	35,963 56,324 25,647 1.00 49,68
ATOM	823 CG PRO 908	37.387 56.216 25.143 1.00 51.43
ATOM	824 C PRO 908	33,852 55.145 25.036 1.00 44.06
ATOM	825 O PRO 908	33.345 55.600 24.008 1.00 44.40
ATOM	826 N GLY 909	33.154 54.772 26.110 1.00 41.44
ATOM	828 CA GLY 909	31.698 54.842 26.135 1.00 37.38
ATOM	829 C GLY 909	30.999 53.502 26.035 1.00 38.26
ATOM	830 O GLY 909	29.778 53.439 25.751 1.00 40.07
ATOM	831 N GLY 910	31.753 52.424 26.264 1.00 36.39
ATOM	833 CA GLY 910	31.178 51.087 26.190 1.00 34.35
ATOM	834 C GLY 910	32.180 49.961 26.360 1.00 31.85
ATOM	835 O GLY 910	33.394 50.235 26.528 1.00 27.95
ATOM	836 N PRO 911	31.710 48.686 26.319 1.00 27.95
ATOM	837 CD PRO 911	30.280 48.339 26.197 1.00 28.51
ATOM	838 CA PRO 911	32.511 47.463 26.467 1.00 25.21
ATOM	839 CB PRO 911	31.438 46.393 26.724 1.00 27.44
ATOM	840 CG PRO 911	30.315 46.840 25.891 1.00 22.45

## FIG. 7(17)

ATOM	841 C PRO 911		25.234 1.00 22.33
ATOM	842 O PRO 911		24.124 1.00 23.57
ATOM	843 N LEU 912	34.548 46.581	
ATOM	845 CA LEU 912	35.412 46.177	
ATOM	846 CB LEU 912	36.778 45.685	24.812 1.00 23.67
ATOM	847 CG LEU 912	38.095 45.759	
ATOM	848 CD1 LEU 912	38.988 44.618	
ATOM	849 CD2 LEU 912	37.906 45.745	
ATOM	850 C LEU 912	34.692 45.010	
ATOM	851 O LEU 912	34.342 44.029	
ATOM	852 N MET 913	34.417 45.142	
ATOM	854 CA MET 913	33.724 44.085	
ATOM	855 CB MET 913	32.264 44.456	
ATOM	856 CG MET 913	31.489 44.461	22.728 1.00 22.26
ATOM	857 SD MET 913	29.829 45.009	22.484 1.00 24.17
ATOM	858 CE MET 913	30.127 46.676	22.205 1.00 20.40
ATOM	859 C MET 913	34.386 43.768	20.295 1.00 20.42
ATOM	860 O MET 913	34.701 44.657	19.519 1.00 21.08
ATOM	861 N VAL 914	34.703 42.491	20.102 1.00 23.72
ATOM	863 CA VAL 914	35.354 42.001	18.891 1.00 20.24
ATOM	864 CB VAL 914	36.614 41.170	19.232 1.00 16.92
ATOM	865 CG1 VAL 914	37.254 40.637	17.958 1.00 19.36
ATOM	866 CG2 VAL 914	37.629 42.055	19.972 1.00 13.30
ATOM	867 C VAL 914	34.296 41.210	18.132 1.00 19.70
ATOM	868 O VAL 914	33.836 40.191	18.587 1.00 26.45
ATOM	869 N ILE 915	33.844 41.775	17.026 1.00 19.86
ATOM	871 CA ILE 915	32.806 41.212	16.179 1.00 20.42
ATOM	872 CB ILE 915	32.034 42.384	15.455 1.00 18.44
ATOM	873 CG2 ILE 915	30.721 41.909	14.869 1.00 12.35
ATOM	874 CG1 ILE 915	31.756 43.531	16.426 1.00 17.60
ATOM	875 CD1 ILE 915	31.358 44.822	15.735 1.00 15.14
ATOM	876 C ILE 915	33.457 40.287	15.115 1.00 23.98
ATOM	877 O ILE 915	34.361 40.722	14.373 1.00 23.30
ATOM	878 N VAL 916	33.054 39.011	15.075 1.00 20.08
ATOM	880 CA VAL 916	33.594 38.089	14.077 1.00 17.64
ATOM	881 CB VAL 916	34.543 37.003	14.680 1.00 9.09
ATOM	882 CG1 VAL 916	35.703 37.685	15.350 1.00 5.05
ATOM	883 CG2 VAL 916	33.817 36.126	15.678 1.00 10.26
ATOM	884 C VAL 916	32.422 37.486	13.342 1.00 17.74
ATOM	885 O VAL 916		
ATOM	886 N GLU 917		12.303 1.00 14.74
ATOM	888 CA GLU 917		11.577 1.00 13.03
<b>ATOM</b>	889 CB GLU 917	32.120 35.409	10.332 1.00 14.06

#### FIG. 7(18)

ATOM 890 CG GLU 917 32,946 36,348 9,464 1,00 24,11 ATOM 891 CD GLU 917 33,543 35,651 8,258 1,00 26,52 33.943 35.651 8.258 1.00 26.52 33.060 35.904 7.139 1.00 27.67 34.480 34.841 8.425 1.00 28.39 30.853 35.051 12.434 1.00 14.78 31.445 34.344 13.234 1.00 14.35 29.557 34.958 12.229 1.00 19.12 ATOM 892 OE1 GLU 917 ATOM 893 OE2 GLU 917 ATOM 894 C GLU 917 ATOM 895 O GLU 917 ATOM 896 N PHE 918 28.688 34.042 12.966 1.00 18.07 27.334 34.721 13.168 1.00 18.48 26.275 33.840 13.748 1.00 17.83 26.328 33.456 15.081 1.00 18.65 ATOM 898 CA PHE 918 ATOM 899 CB PHE 918 ATOM 900 CG PHE 918 ATOM 901 CD1 PHE 918 ATOM 901 CD1 PHE 918
ATOM 902 CD2 PHE 918
ATOM 903 CE1 PHE 918
ATOM 905 CZ PHE 918
ATOM 905 CZ PHE 918
ATOM 906 C PHE 918
ATOM 906 C PHE 918
ATOM 907 O PHE 918
ATOM 908 N CYS 919
ATOM 910 CA CYS 919
ATOM 911 CB CYS 919
ATOM 912 SG CYS 919
ATOM 913 C CYS 919
ATOM 914 O CYS 919 25.213 33.400 12.953 1.00 21.10 25.213 32.639 15.613 1.00 18.12 24.210 32.580 13.473 1.00 14.29 24.274 32.201 14.799 1.00 17.78 28.487 32.805 12.113 1.00 18.83 28.081 32.917 10.964 1.00 11.61 28.761 31.635 12.070 1.00 12.00 28.590 30.372 11.947 1.00 19.00 29.855 29.566 12.069 1.00 16.78 31.225 30.428 11.325 1.00 16.84 28.761 31.635 12.676 1.00 19.49 27.383 29.659 12.550 1.00 21.60 27.474 29.135 13.676 1.00 20.69 26.269 29.653 11.818 1.00 18.06 24.998 29.130 12.318 1.00 28.13 ATOM 914 O CYS 919 ATOM 915 N LYS 920 ATOM 917 CA LYS 920 23.799 29.581 11.459 1.00 25.17 23.595 28.799 10.207 1.00 33.78 22.658 29.509 9.250 1.00 40.32 ATOM 918 CB LYS 920 ATOM 919 CG LYS 920 ATOM 920 CD LYS 920 ATOM 921 CE LYS 920 ATOM 922 NZ LYS 920 ATOM 926 C LVS 927 21.261 29.706 9.829 1.00 51.94 20.343 30.396 8.845 1.00 56.09 24.813 27.679 12.700 1.00 28.53 ATOM 927 O LYS 920 24.020 27.405 13.592 1.00 31.57 928 N PHE 921 25,533 26,757 12,078 1,00 24,89 ATOM 25.328 25.362 12.409 1.00 21.12 25.497 24.518 11.171 1.00 20.75 ATOM 930 CA PHE 921 ATOM 931 CB PHE 921 ATOM 932 CG PHE 921 24,588 24,917 10,084 1,00 22,95 23.224 24.734 10.219 1.00 27.55 25.077 25.564 8.975 1.00 29.40 ATOM 933 CD1 PHE 921 ATOM 934 CD2 PHE 921 22.362 25.205 9.269 1.00 35.42 24.237 26.041 8.013 1.00 32.24 22.869 25.870 8.154 1.00 38.81 26.158 24.823 13.535 1.00 21.23 ATOM 935 CE1 PHE 921 ATOM 936 CE2 PHE 921 ATOM 937 CZ PHE 921 ATOM 938 C PHE 921 ATOM 939 O PHE 921 26,002 23,664 13,900 1,00 22,74

## FIG. 7(19)

ATOM	940 N GLY 922	27.047 25.65	9 14.065	1.00 18.39
ATOM	942 CA GLY 922	27.906 25.25	7 15.172	1.00 17.62
ATOM	943 C GLY 922	29.115 24.45	5 14.759	1.00 18.42
ATOM	944 O GLY 922	29.331 24.23	0 13.581	1.00 20.81
ATOM	945 N ASN 923	29.903 24.01	1 15.729	1.00 22.93
ATOM	947 CA ASN 923	31.092 23.22	3 15.430	1.00 24.85
ATOM	948 CB ASN 923	31.867 22.83	7 16.705	1.00 29.68
ATOM	949 CG ASN 923	31.212 21.71	0 17.493	1.00 39.14
ATOM	950 OD1 ASN 923	31.252 20.55	0 17.087	1.00 41.11
ATOM	951 ND2 ASN 923	30.662 22.03	8 18.660	1.00 35.87
ATOM	954 C ASN 923	30.818 22.01	9 14.523	1.00 21.09
ATOM	955 O ASN 923	29.685 21.56	6 14.370	1.00 20.59
ATOM	956 N LEU 924	31.867 21.52	3 13.896	1.00 21.13
ATOM	958 CA LEU 924	31.740 20.43	1 12.957	1.00 22.85
ATOM	959 CB LEU 924	33.019 20.37	7 12.126	1.00 23.67
ATOM	960 CG LEU 924	33.019 19.46	2 10.920	1.00 17.22
ATOM	961 CD1 LEU 924	31.776 19.69	9 10.125	
ATOM	962 CD2 LEU 924	34.268 19.72	9 10.095	1.00 23.82
ATOM	963 C LEU 924	31.414 19.06	2 13.558	1.00 22.65
ATOM	964 O LEU 924	30.601 18.32	6 13.013	1.00 26.13
ATOM	965 N SER 925	31.035 18.74	2 14.687	
ATOM	967 CA SER 925	31.853 17.46		
ATOM	968 CB SER 925	32.741 17.40		
ATOM	969 OG SER 925	32.426 16.27	2 17.416	1.00 32.86
ATOM	971 C SER 925	30.432 17.21	7 15.812	
ATOM	972 O SER 925	29.863 16.14		
ATOM	973 N THR 926	29.892 18.19		
ATOM	975 CA THR 926	28.535 18.12		
ATOM	976 CB THR 926	28.258 19.33		
ATOM	977 OG1 THR 926	29.230 19.37		
ATOM	979 CG2 THR 926	26.927 19.21		
ATOM	980 C THR 926	27.610 18.04		
ATOM	981 O THR 926	26.654 17.25		
ATOM	982 N TYR 927	27.961 18.76		
ATOM	984 CA TYR 927	27.128 18.71		
ATOM	985 CB TYR 927	27.597 19.72		
ATOM	986 CG TYR 927	26.708 19.68		
ATOM	987 CD1 TYR 927	25.391 20.19		
ATOM	988 CE1 TYR 927	24.567 20.17		
ATOM	989 CD2 TYR 927	27.173 19.13		
ATOM	990 CE2 TYR 927	26.347 19.10		1.00 24.92
ATOM	991 CZ TYR 927	25.058 19.62		1.00 16.40
ATOM	992 OH TYR 927	24.285 19.60	00 7.819	1.00 23.87

#### FIG. 7(20)

FIG. 7(20)

ATOM 994 C TYR 927
ATOM 995 O TYR 927
ATOM 996 N LEU 928
ATOM 999 CA LEU 928
ATOM 999 CB LEU 928
ATOM 1000 CG LEU 928
ATOM 1000 CG LEU 928
ATOM 1001 CD1 LEU 928
ATOM 1002 CD2 LEU 928
ATOM 1003 C LEU 928
ATOM 1004 O LEU 928
ATOM 1005 N ARG 929
ATOM 1007 CA ARG 929
ATOM 1008 CB ARG 929
ATOM 1001 CD ARG 929
ATOM 1010 ARG 929
ATOM 1010 ARG 929
ATOM 1010 ARG 929
ATOM 1011 NE ARG 929
ATOM 1012 CARG 929
ATOM 1013 CARG 929
ATOM 1014 NHI ARG 929
ATOM 1017 NH2 ARG 929
ATOM 1020 C ARG 929
ATOM 1020 C ARG 929
ATOM 1021 O ARG 929
ATOM 1022 N SER 930
ATOM 1024 CA SER 930
ATOM 1025 CB SER 930
ATOM 1026 CS SER 930
ATOM 1027 NE SER 930
ATOM 1030 CB LYS 931
ATOM 1031 CB LYS 931
ATOM 1034 N ARG 932
ATOM 1035 CB LYS 931
ATOM 1034 N ARG 932
ATOM 1035 CB LYS 931
ATOM 1034 N ARG 932
ATOM 1034 N ARG 932
ATOM 1035 CB LYS 931
ATOM 1035 CB LYS 931
ATOM 1035 CB LYS 931
ATOM 1035 N ARG 932
ATOM 1035 CB LYS 931
ATOM 1036 CB LYS 931
ATOM 1037 NA LYS 931
ATOM 1042 C LYS 931
ATOM 1043 N ARG 932
ATOM 1044 O LYS 931
ATOM 1045 N ARG 932
ATOM 1045 N ARG 932
ATOM 1046 N ARG 932
ATOM 1047 NLYS 931
ATOM 1040 N ARG 932
ATOM 1040 N ARG 932
ATOM 1040 N ARG 931
ATOM 1040 N ARG 932
ATOM 1040 N ARG 931
ATOM 1040 N ARG 932
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ATOM 1040 N ARG 932
ATOM 1040 N ARG 932 ATOM 1041 C LYS 931
ATOM 1042 O LYS 931
ATOM 1042 O LYS 931
ATOM 1043 N ARG 932
ATOM 1045 CA ARG 932
ATOM 1045 CA ARG 932
ATOM 1047 CG ARG 932
ATOM 1048 CD ARG 932
ATOM 1049 NE ARG 932
ATOM 1049 NE ARG 932
ATOM 1051 CZ ARG 935

#### FIG. 7(21)

ATOM 1052 NH1 ARG 932 30,018 9,098 15,809 1,00 47,32 ATOM 1055 NH2 ARG 932 27,916 8,725 16,645 1,00 53,04 ATOM 1058 C ARG 932 23,621 9,087 10,273 1,00 41,54 ATOM 1059 O ARG 932 23.821 8.135 9.532 1.00 41.31 ATOM 1060 N ASN 933 22.412 9.582 10.536 1.00 44.37 ATOM 1062 CA ASN 933 21.181 9.069 9.956 1.00 47.14 ATOM 1063 CB ASN 933 19.974 9.453 10.824 1.00 54.55 ATOM 1064 CG ASN 933 19.783 8.545 12.050 1.00 57.14 ATOM 1065 OD1 ASN 933 20.622 7.693 12.369 1.00 54.11 ATOM 1066 ND2 ASN 933 18,668 8,752 12,757 1,00 57,76 ATOM 1069 C ASN 933 20,974 9,680 8,589 1,00 49,60 ATOM 1070 O ASN 933 20.260 9.125 7.753 1.00 55.62 ATOM 1071 N GLU 934 21,494 10,888 8,403 1,00 52,11 ATOM 1073 CA GLU 934 21.365 11.580 7.122 1.00 52.39 ATOM 1074 CB GLU 934 ATOM 1075 CG GLU 934 20.859 13.007 7.323 1.00 56.14 20.859 13.007 7.323 1.00 56.14 19.434 13.095 7.822 1.00 59.40 ATOM 1076 CD GLU 934 ATOM 1077 OE1 GLU 934 ATOM 1078 OE2 GLU 934 ATOM 1079 C GLU 934 ATOM 1080 C GLU 934 19.332 13.686 9.211 1.00 63.97 18.427 13.250 9.953 1.00 69.17 20.138 14.580 9.563 1.00 64.27 22.677-11.593 6.332 1.00 50.45 23,188 12,663 5,961 1,00 50,70 ATOM 1081 N PHE 935 23.205 10.396 6.070 1.00 46.25 ATOM 1083 CA PHE 935 24,440 10,225 5,325 1,00 41,20 ATOM 1084 CB PHE 935 25,638 10,121 6,268 1,00 40,97 ATOM 1085 CG PHE 935 26,923 9,800 5,555 1,00 39,81 ATOM 1086 CD1 PHE 935 27.327 8.478 5.378 1.00 34.65 ATOM 1087 CD2 PHE 935 27,676 10,815 4,970 1,00 33,02 ATOM 1088 CE1 PHE 935 28.455 8.180 4.617 1.00 32.30 ATOM 1089 CE2 PHE 935 28,793 10,515 4,218 1,00 29,96 ATOM 1090 CZ PHE 935 29,181 9,201 4,037 1,00 29,08 ATOM 1091 C PHE 935 24,474 9,006 4,412 1,00 40,49 ATOM 1092 O PHE 935 24.394 7.871 4.865 1.00 40.47 ATOM 1093 N VAL 936 24.694 9.237 3.133 1.00 38.66 ATOM 1095 CA VAL 936 24,809 8,138 2,208 1,00 43,29 ATOM 1096 CB VAL 936 23,663 8.113 1.221 1.00 40,39 ATOM 1097 CG1 VAL 936 23,739 9,312 0,280 1,00 34,50 ATOM 1098 CG2 VAL 936 23,720 6,841 0,444 1,00 42,47 ATOM 1099 C VAL 936 26.087 8.436 1.438 1.00 49.63 ATOM 1100 O VAL 936 26.322 9.585 1.081 1.00 55.64 26.960 7.433 1.222 1.00 50.29 26.966 6.087 1.822 1.00 49.69 26.322 9.585 1.081 1.00 55.64 ATOM 1101 N PRO 937 ATOM 1102 CD PRO 937 ATOM 1103 CA PRO 937 28.207 7.669 0.483 1.00 50.65 ATOM 1104 CB PRO 937 28.676 6.260 0.177 1.00 46.68

## FIG. 7(22)

ATOM	1105 CG PRO 937	28.378 5.582 1.493 1.00 47.42
ATOM	1106 C PRO 937	28.019 8.501 -0.774 1.00 53.83
ATOM	1107 O PRO 937	28.644 9.558 -0.937 1.00 53.64
ATOM	1108 N TYR 938	27.153 8.046 -1.660 1.00 54.91
ATOM	1110 CA TYR 938	26.918 8.803 -2.859 1.00 62.52
ATOM	1111 CB TYR 938	27.580 8.161 -4.080 1.00 67.73
ATOM	1120 C TYR 938	25.443 8.800 -3.059 1.00 67.31
ATOM	1121 O TYR 938	24.722 8.082 -2.361 1.00 66.13
ATOM	1122 N LYS 939	25.027 9.601 -4.038 1.00 75.30
ATOM	1124 CA LYS 939	23.639 9.770 -4.445 1.00 81.21
ATOM	1125 CB LYS 939	23.209 11.254 -4.284 1.00 80.04
ATOM	1126 C LYS 939	23.543 9.331 -5.921 1.00 87.24
ATOM	1127 O LYS 939	24.582 9.384 -6.646 1.00 90.23
ATOM	1129 CB ASP 998	17.986 15.692 3.023 1.00 53.00
ATOM	1130 C ASP 998	20.489 15.723 3.377 1.00 55.33
ATOM	1131 O ASP 998	21.051 16.058 4.426 1.00 56.29
ATOM	1134 N ASP 998	19.408 16.931 1.400 1.00 54.52
ATOM	1136 CA ASP 998	19.279 16.514 2.829 1.00 55.12
ATOM	1137 N PHE 999	20.900 14.687 2.653 1.00 52.90
ATOM	1139 CA PHE 999	21.984 13.834 3.111 1.00 46.86
ATOM	1140 CB PHE 999	21.841 12.420 2.528 1.00 51.05
ATOM	1141 CG PHE 999	20.897 11.537 3.296 1.00 55.62
ATOM	1142 CD1 PHE 999	21.249 10.236 3.606 1.00 56.12
ATOM	1143 CD2 PHE 999	19.671 12.022 3.751 1.00 60.98
ATOM	1144 CE1 PHE 999	20.397 9.422 4.368 1.00 61.93
ATOM	1145 CE2 PHE 999	18.816 11.222 4.509 1.00 61.09
ATOM	1146 CZ PHE 999	19.183 9.917 4.820 1.00 60.64
ATOM	1147 C PHE 999	23.373 14.302 2.837 1.00 41.06
ATOM	1148 O PHE 999	23.632 14.937 1.820 1.00 36.04
ATOM	1149 N LEU 1000	24.238 14.057 3.812 1.00 37.57
ATOM	1151 CA LEU 1000	25.651 14.326 3.652 1.00 36.08
ATOM	1152 CB LEU 1000	26.401 14.306 4.985 1.00 35.67
ATOM	1153 CG LEU 1000	25.923 15.286 6.057 1.00 36.23
ATOM	1154 CD1 LEU 1000	26.941 15.370 7.201 1.00 29.94
ATOM	1155 CD2 LEU 1000	25.707 16.654 5.435 1.00 38.66
ATOM	1156 C LEU 1000	26.089 13.139 2.756 1.00 35.16
ATOM	1157 O LEU 1000	25.330 12.167 2.569 1.00 32.68
ATOM	1158 N THR 1001	27.292 13.228 2.201 1.00 29.92
ATOM	1160 CA THR 1001	27.803 12.236 1.285 1.00 25.42
ATOM	1161 CB THR 1001	27.396 12.560 -0.178 1.00 30.10

## FIG. 7(23)

ATOM	1162 OG1 THR 1001	28.055 13.771 -0.605 1.00 33.54
ATOM	1164 CG2 THR 1001	25.878 12.741 -0.326 1.00 29.24
ATOM	1165 C THR 1001	29.303 12.388 1.338 1.00 27.68
ATOM	1166 O THR 1001	29.805 13.303 1.985 1.00 28.02
ATOM	1167 N LEU 1002	30.020 11.552 0.592 1.00 26.85
ATOM	1169 CA LEU 1002	31.454 11.636 0.572 1.00 24.39
ATOM	1170 CB LEU 1002	32.044 10.545 -0.298 1.00 22.71
ATOM	1171 CG LEU 1002	32.269 9.304 0.573 1.00 27.80
ATOM	1172 CD1 LEU 1002	32.727 8.142 -0.280 1.00 27.11
ATOM	1173 CD2 LEU 1002	33.295 9.592 1.670 1.00 24.64
ATOM	1174 C LEU 1002	31.908 12.995 0.099 1.00 26.97
ATOM	1175 O LEU 1002	32.967 13.459 0.506 1.00 26.84
ATOM	1176 N GLU 1003	31.063 13.682 -0.666 1.00 27.89
ATOM	1178 CA GLU 1003	31.428 15.000 -1.185 1.00 28.02
ATOM	1179 CB GLU 1003	30.419 15.503 -2.208 1.00 32.50
ATOM	1180 CG GLU 1003	30.988 16.624 -3.077 1.00 37.49
ATOM	1181 CD GLU 1003	31.915 16.121 -4.170 1.00 38.89
ATOM	1182 OE1 GLU 1003	33.065 15.743 -3.886 1.00 43.61
ATOM	1183 OE2 GLU 1003	31.488 16.102 -5.331 1.00 46.97
ATOM	1184 C GLU 1003	31.591 16.044 -0.117 1.00 25.24
ATOM	1185 O GLU 1003	32.485 16.885 -0.211 1.00 26.57
ATOM	1186 N HIS 1004	30.748 15.953 0.913 1.00 23.16
ATOM	1188 CA HIS 1004	30.746 16.884 2.040 1.00 19.58
ATOM	1189 CB HIS 1004	29.508 16.719 2.912 1.00 19.12
ATOM	1190 CG HIS 1004	28.227 17.024 2.208 1.00 23.47
ATOM	1191 CD2 HIS 1004	27.173 17.784 2.570 1.00 23.78
ATOM	1192 ND1 HIS 1004	27.911 16.508 0.964 1.00 27.88
ATOM	1194 CE1 HIS 1004	26.718 16.936 0.596 1.00 20.57
ATOM	1195 NE2 HIS 1004	26.246 17.710 1.554 1.00 23.61
ATOM	1197 C HIS 1004	31.940 16.631 2.885 1.00 21.64
ATOM	1198 O HIS 1004	32.753 17.508 3.075 1.00 25.00
ATOM	1199 N LEU 1005	32.055 15.419 3.394 1.00 23.11
ATOM	1201 CA LEU 1005	33.186 15.072 4.222 1.00 23.79
ATOM	1202 CB LEU 1005	33.131 13.581 4.589 1.00 24.17
ATOM	1203 CG LEU 1005	32.183 13.199 5.743 1.00 27.48
ATOM	1204 CD1 LEU 1005	31.030 14.150 5.821 1.00 25.44
ATOM	1205 CD2 LEU 1005	31.679 11.771 5.627 1.00 22.50
ATOM	1206 C LEU 1005	34.506 15.467 3.558 1.00 20.41
ATOM	1207 O LEU 1005	35.361 16.034 4.206 1.00 21.82
ATOM	1208 N ILE 1006	34.668 15.212 2.264 1.00 19.50

## FIG. 7(24)

ATOM	1210 CA ILE 1006	35.914	15.589	1.609	1.00 18.77
ATOM	1211 CB ILE 1006	36.128	14.806	0.276	1.00 16.46
ATOM	1212 CG2 ILE 1006	37.602	14.777	-0.103	1.00 12.82
ATOM	1213 CG1 ILE 1006	35.718	13.341	0.441	1.00 20.16
ATOM	1214 CD1 ILE 1006	35.961	12,446	-0.834	1.00 11.88
ATOM	1215 C ILE 1006	35.998	17.136	1.377	1.00 22.88
ATOM	1216 O ILE 1006	37.113	17,730	1.431	1.00 21.25
ATOM	1217 N CYS 1007	34.854	17.788	1.108	1.00 21.47
ATOM	1219 CA CYS 1007	34.860	19.240	0.909	1.00 21.66
ATOM	1220 CB CYS 1007	33.522	19.825	0.431	1.00 24.87
ATOM	1221 SG CYS 1007	33.760	21.544	-0.085	1.00 30.17
ATOM	1222 C CYS 1007	35.247	19.953	2.196	1.00 22.22
ATOM	1223 O CYS 1007	36.024	20.905	2.158	1.00 25.94
ATOM	1224 N TYR 1008	34.691	19.527	3.331	1.00 20.53
ATOM	1226 CA TYR 1008	35.030	20.132	4.617	1.00 17.94
ATOM	1227 CB TYR 1008	34.248	19.493	5.758	1.00 18.61
ATOM	1228 CG TYR 1008	32.753	19.488	5.626	1.00 17.97
ATOM	1229 CD1 TYR 1008	32.019	18.455	6.175	1.00 16.67
ATOM	1230 CE1 TYR 1008	30.641	18.462	6.158	1.00 22.78
ATOM	1231 CD2 TYR 1008	32.059	20.549	5.031	1.00 22.19
ATOM	1232 CE2 TYR 1008	30.646	20.569	5.011	1.00 20.60
ATOM	1233 CZ TYR 1008	29.949	19.513	5,579	1.00 23.22
ATOM	1234 OH TYR 1008	28.574	19.454	5.551	1.00 18.30
ATOM	1236 C TYR 1008	36.537	19.945	4.883	1.00 18.55
ATOM	1237 O TYR 1008	37.217	20.917	5.256	1.00 20.35
ATOM	1238 N SER 1009	37.056	18.726	4.642	1.00 14.74
ATOM	1240 CA SER 1009	38.476	18.409	4.852	1.00 13.39
ATOM	1241 CB SER 1009	38.810	16.962	4.473	1.00 17.24
ATOM	1242 OG SER 1009	38.018	16.001	5.152	1.00 26.04
ATOM	1244 C SER 1009		19.309		1.00 16.36
ATOM	1245 O SER 1009		19.864		1.00 20.21
ATOM	1246 N PHE 1010		19.375		1.00 20.97
ATOM	1248 CA PHE 1010		20.246		1.00 23.34
ATOM	1249 CB PHE 1010		20.126		1.00 18.83
ATOM	1250 CG PHE 1010		21.002		1.00 17.13
ATOM	1251 CD1 PHE 1010				1.00 13.94
ATOM	1252 CD2 PHE 1010				1.00 17.85
ATOM	1253 CE1 PHE 1010				1.00 16.30
ATOM	1254 CE2 PHE 1010				1.00 17.15
ATOM	1255 CZ PHE 1010	40.772	22.714	-2.608	1.00 18.02

## FIG. 7(25)

ATOM	1256 C PHE 1010	39.688 21.746	2.242 1.00 22.02
ATOM	1257 O PHE 1010	40.749 22.390	2.298 1.00 23.00
ATOM	1258 N GLN 1011	38.535 22.271	2.643 1.00 19.25
ATOM	1260 CA GLN 1011	38.418 23.640	3.159 1.00 19.07
ATOM	1261 CB GLN 1011	36.980 23.945	3.480 1.00 12.84
ATOM	1262 CG GLN 1011	36.117 24.005	2.270 1.00 6.53
ATOM	1263 CD GLN 1011	34.713 24.371	2.659 1.00 18.81
ATOM	1264 OE1 GLN 1011	34.490 25.382	3.347 1.00 21.22
ATOM	1265 NE2 GLN 1011	33.760 23.525	2.302 1.00 26.88
ATOM	1268 C GLN 1011	39.262 23.894	4.394 1.00 18.28
ATOM	1269 O GLN 1011	39.840 24.982	4.543 1.00 19.80
ATOM	1270 N VAL 1012	39.270 22.934	5.319 1.00 11.82
ATOM	1272 CA VAL 1012	40.110 23.063	6.500 1.00 13.54
ATOM	1273 CB VAL 1012	39.825 21.936	7.528 1.00 15.67
ATOM	1274 CG1 VAL 1012	40.686 22.107	8.795 1.00 10.56
ATOM	1275 CG2 VAL 1012	38.370 21.948	7.901 1.00 14.92
ATOM	1276 C VAL 1012	41.618 23.068	6.068 1.00 16.72
ATOM	1277 O VAL 1012	42.448 23.782	6.665 1.00 20.48
ATOM	1278 N ALA 1013	42.001 22.291	5.051 1.00 15.90
ATOM	1280 CA ALA 1013	43.401 22.352	4.602 1.00 17.77
ATOM	1281 CB ALA 1013	43.732 21.206	3.638 1.00 10.59
ATOM	1282 C ALA 1013	43.685 23.755	3.963 1.00 15.74
ATOM	1283 O ALA 1013	44.764 24.302	4.139 1.00 17.49
ATOM	1284 N LYS 1014	42.718 24.342	3.244 1.00 17.18
ATOM	1286 CA LYS 1014	42.866 25.706	2.665 1.00 15.11
ATOM	1287 CB LYS 1014	41.557 26.152	2.020 1.00 23.73
ATOM	1288 CG LYS 1014	41.146 25.474	0.748 1.00 23.57
ATOM	1289 CD LYS 1014	41.963 26.033	-0.354 1.00 26.38
ATOM	1290 CE LYS 1014		-1.617 1.00 38.71
ATOM	1291 NZ LYS 1014		-2.776 1.00 50.36
ATOM	1295 C LYS 1014	43.105 26.678	3.823 1.00 11.16
ATOM	1296 O LYS 1014	44.066 27.452	3.818 1.00 13.85
ATOM	1297 N GLY 1015	42.210 26.590	4.816 1.00 10.82
ATOM	1299 CA GLY 1015	42.250 27.403	6.017 1.00 12.48
ATOM	1300 C GLY 1015	43.584 27.327	6.715 1.00 17.17
ATOM	1301 O GLY 1015	44.124 28.349	7.130 1.00 19.92
ATOM	1302 N MET 1016	44.159 26.128	6.763 1.00 17.82
ATOM	1304 CA MET 1016	45.426 25.927	7.439 1.00 15.78
ATOM	1305 CB MET 1016 -	45.516 24.488	7.925 1.00 17.77
ATOM	1306 CG MET 1016	44.538 24.156	9.057 1.00 15.19
ATOM	1307 SD MET 1016	44.931 24.991	10.623 1.00 15.49

#### FIG. 7(26)

ATOM 1308 CE MET 1016 ATOM 1309 C MET 1016 ATOM 1310 O MET 1016 ATOM 1311 N GLU 1017 ATOM 1313 CA GLU 1017 ATOM 1314 CB GLU 1017 ATOM 1315 CG GLU 1017 ATOM 1316 CD GLU 1017 ATOM 1317 OE1 GLU 1017 ATOM 1318 OE2 GLU 1017 ATOM 1319 C GLU 1017 ATOM 1320 O GLU 1017 ATOM 1321 N PHE 1018 ATOM 1323 CA PHE 1018 ATOM 1324 CB PHE 1018 ATOM 1325 CG PHE 1018 ATOM 1326 CD1 PHE 1018 ATOM 1327 CD2 PHE 1018 ATOM 1328 CE1 PHE 1018 ATOM 1329 CE2 PHE 1018 ATOM 1330 CZ PHE 1018 ATOM 1331 C PHE 1018 ATOM 1332 O PHE 1018 ATOM 1333 N LEU 1019 ATOM 1335 CA LEU 1019 ATOM 1336 CB LEU 1019 ATOM 1337 CG LEU 1019 ATOM 1338 CD1 LEU 1019 ATOM 1339 CD2 LEU 1019 ATOM 1340 C LEU 1019 ATOM 1341 O LEU 1019 ATOM 1342 N ALA 1020 ATOM 1344 CA ALA 1020 ATOM 1345 CB ALA 1020 ATOM 1346 C ALA 1020 ATOM 1347 O ALA 1020 ATOM 1348 N SER 1021 ATOM 1350 CA SER 1021 ATOM 1351 CB SER 1021

46.642 24.894 10.658 1.00 5.63 46.642 24.894 10.658 1.00 5.63 46.625 26.321 6.618 1.00 14.62 47.680 26.667 7.163 1.00 15.76 46.487 26.208 5.305 1.00 14.65 47.552 26.608 4.384 1.00 21.43 47.177 26.195 2.947 1.00 21.43 48.162 26.622 1.878 1.00 22.82 47.634 26.421 0.436 1.00 27.12 46.457 26.769 0.141 1.00 24.95 48.418 25.927 -0.424 1.00 32.93 47.667 28.145 4.535 1.00 18.38 48.760 28.648 4.593 1.00 18.48 48.760 28.668 4.593 1.00 17.43 46.526 28.839 4.677 1.00 19.09 46.509 30.295 4.894 1.00 20.74 45.067 30.848 4.870 1.00 27.18 44.942 32.338 5.248 1.00 25.91 44.477 32.718 6.521 1.00 26.19 45.300 33.345 4.348 1.00 25.16 44.381 34.059 6.890 1.00 27.10 45,208 34,708 4,712 1,00 28,34 44.754 35.064 5.982 1.00 26.60 47.179 30.663 6.216 1.00 18.20 48.139 31.430 6.228 1.00 15.08 46.676 30.122 7.328 1.00 16.94 47.259 30.414 8.654 1.00 19.44 46,673 29,533 9,754 1,00 22,88 45.238 29.773 10.165 1.00 24.41 44.956 28.916 11.388 1.00 24.01 45.238 29.773 10.165 1.00 24.41 45.084 31.277 10.485 1.00 25.61 48,736 30,173 8,660 1,00 19,44 49.493 30.896 9.316 1.00 18.98 49.135 29.076 8.023 1.00 19.45 50.545 28.747 7.961 1.00 22.29 50.748 27.350 7.397 1.00 21.86 51.252 29.829 7.115 1.00 26.13 52,348 30,257 7,471 1,00 25,25 50.600 30.323 6.050 1.00 29.72 51.194 31.384 5.219 1.00 27.59 50.289 31.754 4.026 1.00 23.95

## FIG. 7(27)

ATOM 1352 OG SER 1021 49.252 32.662 4.349 1.00 22.60 51.469 32.614 6.109 1.00 32.83 ATOM 1354 C SER 1021 ATOM 1355 O SER 1021 52.570 33.172 6.073 1.00 36.57 ATOM 1355 O SER 1021 52.570 33.172 6,073 1.00 36.57 ATOM 1356 N ARG 1022 50.645 34.093 7.901 1.00 22.64 ATOM 1359 CB ARG 1022 ATOM 1360 CG ARG 1022 ATOM 1361 CD ARG 1022 ATOM 1362 NE ARG 1022 ATOM 1365 NH1 ATOM 1368 NH2 ARG 1022 48.508 38.620 6.862 1.00 40.00 ATOM 1371 C ARG 1022 51.563 33.787 9.056 1.00 24.84 ATOM 1372 O ARG 1022 51.718 34.612 9.960 1.00 23.27 52.115 32.576 9.061 1.00 23.84 53.039 32.137 10.094 1.00 23.59 ATOM 1373 N LYS 1023 ATOM 1375 CA LYS 1023 ATOM 1376 CB LYS 1023 54.237 33.067 10.196 1.00 22.44 52.404 53.007 10.190 1.00 22.41 52.404 31.899 11.456 1.00 25.21 53.054 32.024 12.504 1.00 28.54 51.164 31.435 11.411 1.00 20.82 50.404 31.114 12.595 1.00 28.12 48.982 31.709 12.472 1.00 30.32 48.936 33.504 12.847 1.00 33.73 50.393 20.576 12.729 1.00 32.20 ATOM 1377 C LYS 1023 ATOM 1378 O LYS 1023 ATOM 1379 N CYS 1024 ATOM 1381 CA CYS 1024 ATOM 1382 CB CYS 1024 ATOM 1383 SG CYS 1024 ATOM 1384 C CYS 1024 50,388 29,576 12,729 1,00 32,20 ATOM 1385 O CYS 1024 50.636 28.882 11.756 1.00 38.70 50.167 29.057 13.934 1.00 30.55 50.123 27.619 14.216 1.00 33.60 51.406 27.169 14.970 1.00 36.10 51.223 25.807 15.619 1.00 38.88 52.585 27.121 13.988 1.00 38.38 53.913 27.422 14.604 1.00 34.51 48.891 27.526 15.104 1.00 33.66 48.751 28.301 16.034 1.00 41.71 47.958 26.643 14.797 1.00 31.27 46.742 26.570 15.589 1.00 27.97 45.691 25.745 14.861 1.00 23.43 44.283 26.091 15.229 1.00 30.06 43.342 26.801 14.560 1.00 33.43 50,636 28,882 11,756 1,00 38,70 ATOM 1386 N ILE 1025 ATOM 1388 CA ILE 1025 ATOM 1389 CB ILE 1025 ATOM 1390 CG2 ILE 1025 ATOM 1391 CG1 ILE 1025 ATOM 1392 CD1 ILE 1025 ATOM 1393 C ILE 1025 ATOM 1394 O ILE 1025 ATOM 1395 N HIS 1026 ATOM 1397 CA HIS 1026 ATOM 1398 CB HIS 1026 ATOM 1399 CG HIS 1026 ATOM 1400 CD2 HIS 1026 43.342 26.801 14.560 1.00 33.43 43.680 25.659 16.393 1.00 24.53 ATOM 1401 ND1 HIS 1026

## FIG. 7(28)

ATOM 1403 CE1 HIS 1026 42,428 26,085 16,424 1,00 26,31 ATOM 1404 NE2 HIS 1026 42.199 26.781 15.321 1.00 29.05 ATOM 1406 C HIS 1026 46.901 26.086 17.036 1.00 30.13 46.335 26.681 17.955 1.00 37.96 47.662 25.024 17.244 1.00 26.58 47.872 24.429 18.583 1.00 31.87 48.235 25.483 19.666 1.00 20.17 46.762 23.449 19.055 1.00 31.55 47.047 22.477 19.742 1.00 38.11 ATOM 1407 O HIS 1026 ATOM 1408 N ARG 1027 ATOM 1410 CA ARG 1027 ATOM 1411 CB ARG 1027 ATOM 1412 C ARG 1027 ATOM 1413 O ARG 1027 ATOM 1414 N ASP 1028 45.528 23.629 18.597 1.00 30.85 44.466 22.698 18.955 1.00 26.34 43.788 23.098 20.248 1.00 32.60 ATOM 1416 CA ASP 1028 ATOM 1417 CB ASP 1028 42.847 22.020 20.755 1.00 35.64 41.602 22.245 ATOM 1418 CG ASP 1028 ATOM 1419 OD1 ASP 1028 ATOM 1420 OD2 ASP 1028 41.692 22.346 21.096 1.00 36.08 43.267 20.842 20.790 1.00 40.39 ATOM 1421 C ASP 1028 ATOM 1422 O ASP 1028 ATOM 1423 N LEU 1029 ATOM 1425 CA LEU 1029 ATOM 1426 CB LEU 1029 43.435 22.565 17.841 1.00 26.23 42.276 22.926 17.998 1.00 23.40 43.884 22.034 16.708 1.00 23.84 43.053 21.842 15.533 1.00 23.16 43.958 21.772 14.299 1.00 18.78 43.221 21.714 12.965 1.00 20.21 ATOM 1427 CG LEU 1029 43.221 21.714 12.965 1.00 20.21 42.349 22.952 12.812 1.00 15.13 ATOM 1428 CD1 LEU 1029 ATOM 1429 CD2 LEU 1029 44,249 21,601 11,827 1,00 22,91 42.237 20.562 15.700 1.00 25.25 42.765 19.473 15.591 1.00 30.47 40.949 20.703 15.957 1.00 25.99 ATOM 1430 C LEU 1029 ATOM 1431 O LEU 1029 ATOM 1432 N ALA 1030
ATOM 1432 N ALA 1030
ATOM 1434 CA ALA 1030
ATOM 1435 CB ALA 1030
ATOM 1435 C B ALA 1030
ATOM 1436 C ALA 1030
ATOM 1437 O ALA 1030
ATOM 1438 N ALA 1031
ATOM 1440 CA ALA 1031
ATOM 1440 CA ALA 1031
ATOM 1441 CB ALA 1031
ATOM 1442 C ALA 1031
ATOM 1444 N ARG 1032
ATOM 1444 N ARG 1032
ATOM 1444 CB ARG 1032
ATOM 1445 CG ARG 1032
ATOM 1446 CA ARG 1032
ATOM 1447 CB ARG 1032
ATOM 1448 CG ARG 1032
ATOM 1449 CD ARG 1032 ATOM 1432 N ALA 1030

## FIG. 7(29)

ATOM 1450 NE ARG 1032 38.554 20.752 21.158 1.00 41.28 39.464 19.799 21.352 1.00 32.28 ATOM 1452 CZ ARG 1032 ATOM 1453 NH1 ARG 1032 40.677 20.129 21.709 1.00 27.74 ATOM 1456 NH2 ARG 1032 39,178 18,524 21,148 1,00 31,24 35.296 22.708 17.482 1.00 25.91 ATOM 1459 C ARG 1032 ATOM 1460 O ARG 1032 34,601 23,605 17,935 1,00 30,23 ATOM 1461 N ASN 1033 36.451 22.911 16.840 1.00 20.90 37.008 24.222 16.495 1.00 15.77 38.497 24.290 16.813 1.00 18.29 ATOM 1463 CA ASN 1033 ATOM 1464 CB ASN 1033 ATOM 1465 CG ASN 1033 38.760 24.160 18.254 1.00 20.60 37.891 24.445 19.067 1.00 29.84 39.929 23.677 18.601 1.00 18.08 38.760 24.160 18.254 1.00 20.60 ATOM 1466 OD1 ASN 1033 ATOM 1467 ND2 ASN 1033 ATOM 1467 ND2 ASN 1033 ATOM 1470 C ASN 1033 ATOM 1471 O ASN 1033 ATOM 1472 N ILE 1034 ATOM 1474 CA ILE 1034 ATOM 1475 CB ILE 1034 ATOM 1475 CG2 ILE 1034 ATOM 1477 CG1 ILE 1034 ATOM 1478 CD1 ILE 1034 36.839 24.535 15.019 1.00 19.29 37.619 25.303 14.450 1.00 17.18 35.934 23.822 14.456 1.00 17.56 35.631 24.092 12.972 1.00 17.92 35.813 22.868 12.091 1.00 15.66 35.364 23.192 10.647 1.00 12.61 37.247 22.349 12.221 1.00 10.8 38.312 23.384 11.994 1.00 18.10 ATOM 1479 C ILE 1034 34.147 24.381 13.075 1.00 21.87 33.410 23.592 13.669 1.00 26.72 33.711 25.524 12.575 1.00 21.91 ATOM 1480 O ILE 1034 ATOM 1481 N LEU 1035 32.311 25.883 12.670 1.00 19.45 32.190 27.310 13.181 1.00 18.73 32.102 27.454 14.691 1.00 21.53 ATOM 1483 CA LEU 1035 ATOM 1484 CB LEU 1035 ATOM 1485 CG LEU 1035 ATOM 1486 CD1 LEU 1035 33.019 26.518 15.456 1.00 8.66 ATOM 1487 CD2 LEU 1035 32,391 28,881 15,016 1,00 19,34 ATOM 1488 C LEU 1035 31,700 25,764 11,316 1,00 20,15 ATOM 1489 O LEU 1035 32.377 25.977 10.310 1.00 21.51 ATOM 1490 N LEU 1036 30.429 25.390 11.275 1.00 24.13 29.745 25.237 10.006 1.00 26.36 29.027 23.882 9.909 1.00 20.57 28.149 23.631 8.681 1.00 17.23 28.877 23.617 7.360 1.00 7.53 ATOM 1492 CA LEU 1036 ATOM 1493 CB LEU 1036 ATOM 1494 CG LEU 1036 ATOM 1495 CD1 LEU 1036 27.566 22.306 8.900 1.00 18.85 28.827 26.432 9.755 1.00 31.45 ATOM 1496 CD2 LEU 1036 ATOM 1497 C LEU 1036 27.953 26.794 10.557 1.00 29.93 29.094 27.061 8.628 1.00 34.52 28.410 28.248 8.215 1.00 37.11 ATOM 1498 O LEU 1036 ATOM 1499 N SER 1037 ATOM 1501 CA SER 1037

## FIG. 7(30)

ATOM	1502 CB SER 1037	29.448 29.220	7.632 1.00 41.11
ATOM	1503 OG SER 1037	28.879 30.439	7.193 1.00 44.80
ATOM	1505 C SER 1037	27.367 27.890	7.209 1.00 39.39
ATOM	1506 O SER 1037	27.045 26.735	7.024 1.00 42.14
ATOM	1507 N GLU 1038	26.884 28.912	6.531 1.00 44.94
ATOM	1509 CA GLU 1038	25.845 28.806	5.534 1.00 50.37
ATOM	1510 CB GLU 1038	25.685 30.152	4.792 1.00 56.15
ATOM	1511 CG GLU 1038	25.599 31.391	5.676 1.00 55.19
ATOM	1512 CD GLU 1038	24.518 31.270	6.708 1.00 59.42
ATOM	1513 OE1 GLU 1038	23.464 30.637	6.419 1.00 58.62
ATOM	1514 OE2 GLU 1038	24.736 31.806	7.816 1.00 63.52
ATOM	1515 C GLU 1038	25.954 27.672	4.518 1.00 51.35
ATOM	1516 O GLU 1038	25.619 26.521	4.816 1.00 57.04
ATOM	1517 N LYS 1039	26.414 27.997	3.317 1.00 46.28
ATOM	1519 CA LYS 1039	26.467 27.021	2.251 1.00 43.05
ATOM	1520 CB LYS 1039	26.455 27.729	0.898 1.00 41.05
ATOM	1521 C LYS 1039	27.689 26.155	2.401 1.00 44.31
ATOM	1522 O LYS 1039	28.687 26.358	1.697 1.00 50.06
ATOM	1523 N ASN 1040	27.611 25.210	3.339 1.00 37.02
ATOM	1525 CA ASN 1040	28.701 24.283	3.630 1.00 32.65
ATOM	1526 CB ASN 1040	28.647 23.041	2.761 1.00 31.69
ATOM	1527 CG ASN 1040	27.641 22.061	3.267 1.00 31.29
ATOM	1528 OD1 ASN 1040	26.740 21.693	2.553 1.00 38.80
ATOM	1529 ND2 ASN 1040	27.749 21.680	4.530 1.00 36.05
ATOM	1532 C ASN 1040	30.096 24.844	3.656 1.00 28.45
ATOM	1533 O ASN 1040	31.079 24.162	3.300 1.00 26.00
ATOM	1534 N VAL 1041	30.174 26.101	4.073 1.00 23.77
ATOM	1536 CA VAL 1041	31.447 26.739	4.207 1.00 16.56
ATOM	1537 CB VAL 1041	31.382 28.274	3.940 1.00 16.16
ATOM	1538 CG1 VAL 1041	32.709 28.948	4.315 1.00 8.57
ATOM	1539 CG2 VAL 1041	31.124 28.509	2.470 1.00 6.79
ATOM	1540 C VAL 1041	31.726 26.382	5.646 1.00 15.50
ATOM	1541 O VAL 1041	30.825 26.333	6.485 1.00 9.73
ATOM	1542 N VAL 1042	32.967 26.022	5.883 1.00 18.82
ATOM	1544 CA VAL 1042	33.431 25.607	7.185 1.00 19.76
ATOM	1545 CB VAL 1042	33.907 24.110	7.051 1.00 22.19
ATOM	1546 CG1 VAL 1042	35.439 23.993	7.041 1.00 18.66
ATOM	1547 CG2 VAL 1042	33.247 23.242	8.100 1.00 22.95
ATOM	1548 C VAL 1042	34.580 26.607	7.483 1.00 20.50
ATOM	1549 O VAL 1042	35.348 26.960	6.575 1.00 17.75

## FIG. 7(31)

ATOM 1550 N LYS 1043 34.675 27.082 8.726 1.00 18.30 ATOM 1552 CA LVS 1043 35,679 28,070 9,103 1,00 17,43 ATOM 1553 CB LYS 1043 34,977 29,420 9,277 1,00 17,68 ATOM 1554 CG LYS 1043 34,202 29,845 8,031 1,00 19,19 ATOM 1555 CD LYS 1043 33,560 31,228 8,186 1,00 26,86 ATOM 1556 CE LYS 1043 33,270 31,885 6,820 1,00 18,32 ATOM 1557 NZ LYS 1043 34,353 32,806 6,425 1,00 22,63 ATOM 1561 C LYS 1043 36.373 27.687 10.399 1.00 18.35 ATOM 1562 O LYS 1043 35,709 27,235 11,330 1,00 17,37 ATOM 1563 N ILE 1044 37.692 27.880 10.461 1.00 17.47 38.504 27.558 11.645 1.00 21.49 40.010 27.390 11.267 1.00 20.48 37,692 27,880 10,461 1,00 17,47 ATOM 1565 CA ILE 1044 ATOM 1566 CB ILE 1044 ATOM 1567 CG2 ILE 1044 40.896 27.250 12.502 1.00 15.75 ATOM 1568 CG1 ILE 1044 40.221 26.237 10.300 1.00 14.66 ATOM 1569 CD1 ILE 1044 41.584 26,344 9,669 1,00 12,76 ATOM 1570 C ILE 1044 38.432 28.735 12.626 1.00 30.73 38.370 29.888 12.207 1.00 31.68 38.454 28.436 13.918 1.00 38.50 38.437 29.444 14.968 1.00 48.73 37.027 29.586 15.558 1.00 50.35 ATOM 1571 O ILE 1044 ATOM 1572 N CYS 1045 ATOM 1574 CA CYS 1045 ATOM 1575 CB CYS 1045 37.027 29.586 15.558 1.00 50.35 ATOM 1576 SG CYS 1045 36.259 28.069 16.173 1.00 59.69 ATOM 1577 C CYS 1045 39,473 29,041 16,033 1,00 54,63 ATOM 1578 O CYS 1045 39,981 27,912 15,986 1,00 54,88 ATOM 1579 N ASP 1046 39.811 29.954 16.956 1.00 64.20 39.811 29.954 16.956 1.00 64.20 40.816 29.700 18.021 1.00 69.98 ATOM 1581 CA ASP 1046 ATOM 1582 CB ASP 1046 40.454 28.407 18.788 1.00 72.94 ATOM 1583 CG ASP 1046 41.338 28.165 20.009 1.00 75.40 ATOM 1584 OD1 ASP 1046 40.930 28.584 21.110 1.00 77.66 ATOM 1585 OD2 ASP 1046 42,428 27,547 19,878 1,00 75,18 ATOM 1586 C ASP 1046 42.219 29.580 17.354 1.00 74.21 ATOM 1587 O ASP 1046 43.183 29.036 17.940 1.00 74.94 42.307 30.205 16.171 1.00 75.46 ATOM 1588 N PHE 1047 ATOM 1590 CA PHE 1047 43.462 30.212 15.245 1.00 71.53 ATOM 1591 CB PHE 1047 42,919 30,267 13,790 1,00 72,10 41.906 31.381 13.526 1.00 71.34 42.139 32.327 12.526 1.00 74.26 ATOM 1592 CG PHE 1047 ATOM 1593 CD1 PHE 1047 42.139 32.321 12.320 100 73.20 40.747 31.501 14.284 1.00 69.46 41.242 33.367 12.293 1.00 70.87 39.847 32.533 14.066 1.00 67.97 40.096 33.467 13.068 1.00 71.41 ATOM 1594 CD2 PHE 1047 ATOM 1595 CE1 PHE 1047 ATOM 1596 CE2 PHE 1047 ATOM 1597 CZ PHE 1047

#### FIG. 7(32)

ATOM 1598 C PHE 1047 44.681 31.163 15.426 1.00 67.78 44.507 32.345 15.797 1.00 63.26 ATOM 1601 CB ASP 1064
ATOM 1602 CG ASP 1064
ATOM 1602 CG ASP 1064
ATOM 1603 OD1 ASP 1064
ATOM 1604 OD2 ASP 1064
ATOM 1605 C ASP 1064
ATOM 1606 O ASP 1064
ATOM 1606 O ASP 1064
ATOM 1609 N ASP 1064
ATOM 1610 CA ASP 1064
ATOM 1611 CA ASP 1064
ATOM 1612 N ALA 1065
ATOM 1615 CB ALA 1065
ATOM 1616 C ALA 1065
ATOM 1616 C ALA 1065
ATOM 1617 O ALA 1065
ATOM 1618 N ARG 1066
ATOM 1620 CA ARG 1066
ATOM 1620 CA ARG 1066
ATOM 1621 CB ARG 1066
ATOM 1623 CD ARG 1066
ATOM 1623 CD ARG 1066
ATOM 1624 NE ARG 1066
ATOM 1624 NE ARG 1066
ATOM 1625 CR ARG 1066
ATOM 1627 NH 1 ARG 1066
ATOM 1628 NH1 ARG 1066
ATOM 1629 CR ARG 1066
ATOM 1620 CH ARG 1066
ATOM 1621 CB ARG 1066
ATOM 1623 CD ARG 1066
ATOM 1624 NE ARG 1066
ATOM 1625 CR ARG 1066
ATOM 1626 CZ ARG 1066
ATOM 1627 NH 1 ARG 1066
ATOM 1628 NH1 ARG 1066
ATOM 1629 CR ARG 1066
ATOM 1629 CR ARG 1066
ATOM 1624 NE ARG 1066
ATOM 1625 NH1 ARG 1066
ATOM 1626 CZ ARG 1066
ATOM 1627 NH 1 ARG 1066
ATOM 1627 NH 1 ARG 1066
ATOM 1627 NH 1 ARG 1066
ATOM 1627 NH1 ARG 1066
ATOM 1628 NH2 ARG 1066
ATOM 1627 NH1 ARG 1066
ATOM 1628 NH2 ARG 1066
ATOM 1629 NH2 ARG 1066
ATOM 1620 NH2 ARG 1066
ATOM 1621 NH1 ARG 1066
ATOM 1627 NH1 ARG 1066
ATOM 1628 NH2 ARG 1066
ATOM 1629 NH2 ARG 1066 ATOM 1599 O PHE 1047 ATOM 1618 N ARG 1066 ATOM 1620 CA ARG 1066 ATOM 1621 CB ARG 1066 ATOM 1622 CG ARG 1066 ATOM 1623 CD ARG 1066 ATOM 1624 NE ARG 1066 ATOM 1630 NH2 ARG 1066 37.046 17.691 18.385 1.00 40.52 ATOM 1633 C ARG 1066 38.428 16.513 25.427 1.00 49.01 ATOM 1634 O ARG 1066 38.652 17.274 26.364 1.00 46.29 ATOM 1635 N LEU 1067 39.251 15.546 25.041 1.00 46.48 ATOM 1637 CA LEU 1067 40.510 15.320 25.709 1.00 45.53 ATOM 1639 CG LEU 1067 41.335 13.549 26.073 1.00 45.53 41.335 13.519 27.441 1.00 44.07 41.335 13.519 27.441 1.00 44.07
42.236 12.322 27.273 1.00 37.52
42.109 14.710 28.057 1.00 39.60
41.530 15.778 24.677 1.00 42.00
41.983 15.010 23.832 1.00 41.05
41.854 17.072 24.698 1.00 41.05
41.265 18.104 25.584 1.00 34.16
42.817 17.661 23.761 1.00 38.41
42.919 19.104 24.277 1.00 36.08 ATOM 1640 CD1 LEU 1067 ATOM 1641 CD2 LEU 1067 ATOM 1642 C LEU 1067 ATOM 1643 O LEU 1067 ATOM 1644 N PRO 1068 ATOM 1645 CD PRO 1068 ATOM 1646 CA PRO 1068 ATOM 1647 CB PRO 1068 ATOM 1648 CG PRO 1968 - 41.496 19.355 24.828 1.00 29.23 ATOM 1649 C PRO 1068 44.197 16.961 23.571 1.00 35.36

## FIG. 7(33)

ATOM 1650 O PRO 1068 44.932 17.258 22.623 1.00 37.80 44.552 16.040 24.455 1.00 33.98 ATOM 1651 N LEU 1069 ATOM 1653 CA LEU 1069 45.829 15.337 24.333 1.00 35.06 46.092 14.517 25.601 1.00 37.80 47.228 13.497 25.488 1.00 40.67 48.599 14.156 25.752 1.00 36.35 ATOM 1654 CB LEU 1069 ATOM 1655 CG LEU 1069 ATOM 1656 CD1 LEU 1069 46.399 12.333 26.445 1.00 40.75 45.776 14.397 23.121 1.00 34.16 46.787 14.115 22.461 1.00 32.14 ATOM 1657 CD2 LEU 1069
ATOM 1658 C LEU 1069
ATOM 1658 O LEU 1069
ATOM 1659 O LEU 1069
ATOM 1660 N LYS 1070
ATOM 1662 CA LYS 1070
ATOM 1663 CB LYS 1070
ATOM 1665 CD LYS 1070
ATOM 1665 CD LYS 1070
ATOM 1666 CE LYS 1070
ATOM 1667 NZ LYS 1070
ATOM 1671 C LYS 1070
ATOM 1673 N TRP 1071
ATOM 1673 N TRP 1071
ATOM 1675 CA TRP 1071
ATOM 1676 CB TRP 1071 ATOM 1657 CD2 LEU 1069 46.787 14.115 22.461 1.00 32.14
44.571 13.916 22.859 1.00 28.95
44.280 13.014 21.765 1.00 28.17
42.828 12.569 21.911 1.00 22.17
42.553 11.730 23.144 1.00 22.02
41.085 11.317 23.107 1.00 24.17
40.851 9.908 23.646 1.00 29.35
39.444 9.436 23.439 1.00 35.82
44.518 13.582 20.340 1.00 29.26
44.368 12.867 19.344 1.00 27.81
44.862 14.865 20.260 1.00 27.00
45.086 15.550 18.995 1.00 27.37
44.191 16.827 18.882 1.00 20.67
42.724 16.551 18.545 1.00 20.12
41.685 16.138 19.451 1.00 17.97
40.524 15.892 18.675 1.00 13.02
41.628 15.944 20.838 1.00 23.76 ATOM 1676 CB TRP 1071 ATOM 1677 CG TRP 1071 ATOM 1678 CD2 TRP 1071 ATOM 1679 CE2 TRP 1071 40.524 15.892 18.675 1.00 13.02 41.628 15.944 20.838 1.00 23.76 42.153 16.560 17.304 1.00 19.50 40.834 16.155 17.373 1.00 13.62 39.342 15.465 19.233 1.00 16.22 40.439 15.511 21.396 1.00 20.67 ATOM 1680 CE3 TRP 1071 ATOM 1681 CD1 TRP 1071 ATOM 1682 NE1 TRP 1071 ATOM 1684 CZ2 TRP 1071 ATOM 1685 CZ3 TRP 1071 ATOM 1685 CZ3 TRP 1071
ATOM 1686 CH2 TRP 1071
ATOM 1687 C TRP 1071
ATOM 1688 O TRP 1071
ATOM 1688 O TRP 1071
ATOM 1698 N MET 1072
ATOM 1691 CA MET 1072
ATOM 1692 CB MET 1072
ATOM 1693 CG MET 1072
ATOM 1694 SD MET 1072
ATOM 1695 CE MET 1072
ATOM 1695 CE MET 1072
ATOM 1696 C MET 1072
ATOM 1696 C MET 1072
ATOM 1697 O MET 1072

## FIG. 7(34)

ATOM 1698 N ALA 1073
ATOM 1700 CA ALA 1073
ATOM 1701 CB ALA 1073
ATOM 1701 CB ALA 1073
ATOM 1702 C ALA 1073
ATOM 1704 N PRO 1074
ATOM 1705 CD PRO 1074
ATOM 1707 CB PRO 1074
ATOM 1707 CB PRO 1074
ATOM 1708 CG PRO 1074
ATOM 1709 C PRO 1074
ATOM 1710 O PRO 1074
ATOM 1710 O PRO 1074
ATOM 1711 N GLU 1075
ATOM 1715 CG GLU 1075
ATOM 1716 CG GLU 1075
ATOM 1717 OEI GLU 1075
ATOM 1718 OE2 GLU 1075
ATOM 1719 C GLU 1075
ATOM 1719 C GLU 1075
ATOM 1712 CA THE 1076
ATOM 1721 N THR 1076
ATOM 1721 N THR 1076
ATOM 1721 CR THE 1076
ATOM 1721 CR THE 1076
ATOM 1721 CR THE 1076
ATOM 1723 CA THE 1076
ATOM 1724 CB THE 1076 ATOM 1723 CA THR 1076 54.304 17.923 21.283 1.00 46.22 52.991 18.319 20.605 1.00 43.95 ATOM 1724 CB THR 1076 ATOM 1724 CB 1HR 1076
ATOM 1725 OG1 THR 1076
ATOM 1727 CG2 THR 1076
ATOM 1728 C THR 1076
ATOM 1729 O THR 1076
ATOM 1730 N ILE 1077

52.991 18.319 20.002 1.00 45.46
53.245 18.666 19.230 1.00 45.93
53.245 18.666 19.230 1.00 45.93
53.991 17.378 22.662 1.00 47.62
54.175 18.057 23.650 1.00 52.45
54.175 18.057 23.650 1.00 52.45
53.442 16.173 22.717 1.00 47.96 ATOM 1730 N ILE 1077
ATOM 1732 CA ILE 1077
ATOM 1733 CB ILE 1077
ATOM 1735 CGI ILE 1077
ATOM 1736 CDI ILE 1077
ATOM 1736 CDI ILE 1077
ATOM 1737 C ILE 1077
ATOM 1737 C ILE 1077
ATOM 1738 O ILE 1077
ATOM 1739 N PHE 1078
ATOM 1741 CA PHE 1078
ATOM 1742 CB PHE 1078
ATOM 1743 CG PHE 1078
ATOM 1743 CG PHE 1078
ATOM 1743 CG PHE 1078
ATOM 1744 CG PHE 1078
ATOM 1745 CG PHE 1078
ATOM 1746 CB PHE 1078
ATOM 1747 CG PHE 1078
ATOM 1748 CG PHE 1078
ATOM 1748 CG PHE 1078
ATOM 1749 CG PHE 1078
ATOM 1740 CG PHE 1078
ATOM 1741 CA PHE 1078
ATOM 1741 CA PHE 1078
ATOM 1742 CB PHE 1078
ATOM 1743 CG PHE 1078
ATOM 1744 CG PHE 1078
ATOM 1745 CG PHE 1078

#### FIG. 7(35)

ATOM 1744 CD1 PHE 1078
ATOM 1745 CD2 PHE 1078
ATOM 1745 CD2 PHE 1078
ATOM 1746 CEI PHE 1078
ATOM 1747 CE2 PHE 1078
ATOM 1748 CZ PHE 1078
ATOM 1748 CZ PHE 1078
ATOM 1749 C PHE 1078
ATOM 1750 O PHE 1078
ATOM 1751 N ASP 1079
ATOM 1751 N ASP 1079
ATOM 1755 CA ASP 1079
ATOM 1755 CG ASP 1079
ATOM 1755 CO ASP 1079
ATOM 1755 CA ARG 1080
ATOM 1750 O ARG 1080
ATOM 1760 N ARG 1080
ATOM 1760 CA ARG 1080
ATOM 1777 CA VAL 1081
ATOM 1780 CB VAL 1081
ATOM 1780 CB VAL 1081
ATOM 1780 CG VAL 1081
ATOM 1783 C A TYR 1082
ATOM 1780 CG TYR 1082
ATOM 1780 CD TYR 1082
ATOM 1780 CD TYR 1082
ATOM 1790 CD1 TYR 1082
ATOM 1790 CD1 TYR 1082
ATOM 1790 CD1 TYR 1082
ATOM 1790 CD2 TYR 1082
ATOM 1791 CEI TYR 1082
ATOM 1792 CD2 TYR 1082
ATOM 1791 CEI TYR 1082
ATOM 1792 CD2 TYR 1082 ATOM 1744 CD1 PHE 1078 56.068 11.612 23.169 1.00 54.09

#### FIG. 7(34)

ATOM 1698 N ALA 1073 50.545 15.800 18.547 1.00 25.55 ATOM 1700 CA ALA 1073 51.571 15.024 17.874 1.00 29.80 ATOM 1701 CB ALA 1073 52,369 15,912 16,958 1,00 22,65 ATOM 1702 C ALA 1073 52,448 14,453 18,989 1.00 34,88 ATOM 1703 O ALA 1073 52.431 14,970 20.115 1.00 39.38 53,183 13,355 18,724 1.00 36.01 ATOM 1704 N PRO 1074 53,087 12,450 17,570 1,00 31,55 ATOM 1705 CD PRO 1074 ATOM 1706 CA PRO 1074 54,040 12,771 19,769 1,00 36,24 54.544 11.485 19.115 1.00 34.34 ATOM 1707 CB PRO 1074 ATOM 1708 CG PRO 1074 53.415 11.137 18.193 1.00 31.88 ATOM 1709 C PRO 1074 55.189 13.670 20.288 1.00 37.13 ATOM 1710 O PRO 1074 55.570 13.575 21.447 1.00 34.58 ATOM 1711 N GLU 1075 55.746 14.533 19.440 1.00 37.40 56.813 15.422 19.884 1.00 40.62 ATOM 1713 CA GLU 1075 57.598 15.990 18.707 1.00 33.55 ATOM 1714 CB GLU 1075 ATOM 1715 CG GLU 1075 56,853 16,957 17,844 1,00 39,40 ATOM 1716 CD GLU 1075 55.952 16.300 16.828 1.00 43.14 ATOM 1717 OE1 GLU 1075 55.965 15.055 16.720 1.00 49.09 55,228 17,040 16,124 1,00 44,63 ATOM 1718 OE2 GLU 1075 56,239 16,546 20,757 1,00 42,73 ATOM 1719 C GLU 1075 56.903 17.061 21.639 1.00 44.76 ATOM 1720 O GLU 1075 ATOM 1721 N THR 1076 54,982 16,888 20,524 1,00 46,13 ATOM 1723 CA THR 1076 54.304 17.923 21.283 1.00 46.22 ATOM 1724 CB THR 1076 52,991 18,319 20,605 1,00 43,95 ATOM 1725 OG1 THR 1076 53.245 18.666 19.230 1.00 46.46 ATOM 1727 CG2 THR 1076 52,361 19,481 21,334 1,00 43,93 ATOM 1728 C THR 1076 53,991 17,378 22,662 1,00 47,62 ATOM 1729 O THR 1076 54,175 18,057 23,650 1,00 52,45 53,442 16,173 22,717 1.00 47,96 ATOM 1730 N ILE 1077 ATOM 1732 CA ILE 1077 53,123 15,528 23,980 1,00 46,99 ATOM 1733 CB ILE 1077 52.496 14.151 23.720 1.00 46.43 52,691 13,232 24,895 1,00 46,16 ATOM 1734 CG2 ILE 1077 51,024 14,306 23,384 1,00 44,29 ATOM 1735 CG1 ILE 1077 ATOM 1736 CD1 ILE 1077 50.336 13.010 23.163 1.00 46.43 ATOM 1737 C ILE 1077 54.418 15.345 24.767 1.00 51.37 ATOM 1738 O ILE 1077 54.473 15.577 25.974 1.00 52.53 55,458 14,931 24,058 1,00 53,41 ATOM 1739 N PHE 1078 56,750 14,696 24,672 1,00 58,94 ATOM 1741 CA PHE 1078 57.506 13.570 23.925 1.00 60.74 ATOM 1742 CB PHE 1078 ATOM 1743 CG PHE 1078 56,901 12,184 24,124 1,00 57,84

#### FIG. 7(35)

ATOM 1744 CD1 PHE 1078 ATOM 1745 CD2 PHE 1078 ATOM 1746 CE1 PHE 1078 ATOM 1747 CE2 PHE 1078 ATOM 1748 CZ PHE 1078 ATOM 1749 C PHE 1078 ATOM 1750 O PHE 1078 ATOM 1751 N ASP 1079 ATOM 1753 CA ASP 1079 ATOM 1754 CB ASP 1079 ATOM 1755 CG ASP 1079 ATOM 1756 OD1 ASP 1079 ATOM 1757 OD2 ASP 1079 ATOM 1758 C ASP 1079 ATOM 1759 O ASP 1079 ATOM 1760 N ARG 1080 ATOM 1762 CA ARG 1080 ATOM 1763 CB ARG 1080 ATOM 1764 CG ARG 1080 ATOM 1765 CD ARG 1080 ATOM 1766 NE ARG 1080 ATOM 1768 CZ ARG 1080 ATOM 1769 NH1 ARG 1080 ATOM 1772 NH2 ARG 1080 ATOM 1775 C ARG 1080 ATOM 1776 O ARG 1080 ATOM 1777 N VAL 1081 ATOM 1779 CA VAL 1081 ATOM 1780 CB VAL 1081 ATOM 1781 CG1 VAL 1081 ATOM 1782 CG2 VAL 1081 ATOM 1783 C VAL 1081 ATOM 1784 O VAL 1081 ATOM 1785 N TYR 1082 ATOM 1787 CA TYR 1082 ATOM 1788 CB TYR 1082 ATOM 1789 CG TYR 1082 ATOM 1790 CD1 TYR 1082 ATOM 1791 CE1 TYR 1082 ATOM 1792 CD2 TYR 1082

56.068 11.612 23.169 1.00 54.09 57,127 11,483 25,298 1,00 58,64 55,478 10,380 23,381 1,00 53,82 56,539 10,254 25,514 1,00 57,20 55,711 9,703 24,555 1,00 55,07 57,574 15,981 24,767 1.00 63.98 57.433 16.738 25.736 1.00 67.06 58.356 16.274 23.724 1.00 66.97 59.215 17.472 23.678 1.00 68.09 60.225 17.402 22.501 1.00 66.89 60.174 16.082 21.714 1.00 69.02 60.254 16.156 20.474 1.00 71.23 60.089 14.980 22.308 1.00 69.71 58.434 18.806 23.599 1.00 67.74 59.011 19.848 23.266 1.00 66.85 57.137 18.747 23.926 1.00 68.20 56,173 19,858 23,898 1.00 66,60 55.997 20.496 25.279 1.00 67.64 54.529 20.758 25.638 1.00 71.26 53,823 19,481 26,096 1,00 73,66 53.823 19.481 26.096 1.00 73.66 52.364 19.610 26.226 1.00 75.75 51.642 18.981 27.157 1.00 74.86 50.321 19.134 27.211 1.00 69.96 50.321 19.134 27.211 1.00 69.96 52.247 18.212 28.060 1.00 72.78 56,305 20,920 22,801 1,00 63,93 55.861 22.069 22.955 1.00 61.93 56,863 20,510 21,667 1,00 61,30 57.034 21.413 20.545 1.00 58.53 58.202 20.951 19.584 1.00 60.54 59,304 20,266 20,370 1.00 62,35 57.701 20.043 18.455 1.00 55.04 55.713 21.481 19.771 1.00 56.90 55.052 20.452 19.560 1.00 57.43 55.287 22.699 19.435 1.00 51.51 54.078 22.909 18.641 1.00 41.08 53.092 23.847 19.332 1.00 37.59 52,275 23,238 20,442 1,00 32,41 52.800 23.135 21.721 1.00 38.13 52.043 22.663 22.781 1.00 38.73 50 961 22.843 20.234 1.00 27.91 50.961 22.843 20.234 1.00 27.91

#### FIG. 7(36)

ATOM 1793 CE2 TYR 1082 50.189 22.374 21.287 1.00 33.59 ATOM 1794 CZ TYR 1082 50.739 22.290 22.572 1.00 36.82 ATOM 1795 OH TYR 1082 50.001 21.874 23.679 1.00 39.60 ATOM 1797 C TYR 1082 54,591 23,598 17,410 1,00 34,81 55.789 21.598 13.837 1.00 29.46 57.150 22.894 14.384 1.00 29.46 ATOM 1798 O TYR 1082 ATOM 1799 N THR 1083 ATOM 1801 CA THR 1083 ATOM 1802 CB THR 1083 ATOM 1803 OG1 THR 1083 ATOM 1805 CG2 THR 1083 ATOM 1806 C THR 1083 53.678 23.371 13.946 1.00 27.79 ATOM 1807 O THR 1083 52.651 22.777 14.293 1.00 28.80 53.804 23.869 12.721 1.00 24.37 52.700 23.615 11.797 1.00 27.69 52.739 24.381 10.465 1.00 28.65 ATOM 1808 N ILE 1084 ATOM 1810 CA ILE 1084 ATOM 1811 CB ILE 1084 ATOM 1812 CG2 ILE 1084 51,450 25,166 10,284 1.00 29,19 ATOM 1813 CG1 ILE 1084 53,977 25.259 10.361 1.00 37.75 55.235 24.517 9.985 1.00 46.61 52.689 22.143 11 450 1.00 26 ATOM 1814 CD1 ILE 1084 52.689 22.143 11.459 1.00 26.44 ATOM 1815 C ILE 1084 ATOM 1816 O ILE 1084 51,627 21,589 11,173 1,00 24,29 53,861 21.507 11.518 1.00 25.11 53,920 20.097 11.188 1.00 24.39 ATOM 1817 N GLN 1085 ATOM 1819 CA GLN 1085 55.315 19.612 10.823 1.00 27.61 55.753 20.012 9.411 1.00 33.25 54.653 19.826 8.347 1.00 34.07 53.943 20.779 8.004 1.00 41.60 ATOM 1820 CB GLN 1085 ATOM 1821 CG GLN 1085 ATOM 1822 CD GLN 1085 ATOM 1823 OE1 GLN 1085 ATOM 1824 NE2 GLN 1085 54,546 18,632 7,797 1,00 28,88 ATOM 1827 C GLN 1085 53,296 19,267 12,258 1,00 23,23 ATOM 1828 O GLN 1085 52,900 18,141 11,981 1,00 25,97 52.900 18.141 11.981 1.00 25.97
53.195 19.798 13.480 1.00 20.86
52.488 19.040 14.507 1.00 18.08
53.044 19.256 15.926 1.00 20.91
52.870 20.559 16.440 1.00 21.60
50.962 19.336 14.353 1.00 20.67
50.138 18.531 14.806 1.00 13.79
50.602 20.415 13.609 1.00 18.68
49.190 20.793 13.324 1.00 11.08
49.038 22.249 12.805 1.00 21.08
48.845 23.287 13.920 1.00 23.79
49.348 24.407 13.745 1.00 31.01 ATOM 1829 N SER 1086 ATOM 1831 CA SER 1086 ATOM 1832 CB SER 1086 ATOM 1833 OG SER 1086 ATOM 1835 C SER 1086 ATOM 1836 O SER 1086 ATOM 1837 N ASP 1087 ATOM 1839 CA ASP 1087 ATOM 1840 CB ASP 1087 ATOM 1841 CG ASP 1087 ATOM 1842 OD1 ASP 1087

#### FIG. 7(37)

48.212 23.013 14.967 1.00 28.91 ATOM 1843 OD2 ASP 1087 48.632 19.860 12.261 1.00 11.16 ATOM 1844 C ASP 1087 47.406 19.640 12.177 1.00 12.65 ATOM 1845 O ASP 1087 49,520 19,390 11,390 1.00 9.61 ATOM 1846 N VAL 1088 ATOM 1848 CA VAL 1088 49.181 18.404 10.345 1.00 13.37 ATOM 1849 CB VAL 1088 50.351 18.195 9.389 1.00 15.40 ATOM 1850 CG1 VAL 1088 50.057 17.067 8.486 1.00 14.68 ATOM 1851 CG2 VAL 1088 50.609 19.477 8.587 1.00 10.67 48.839 17.061 11.014 1.00 13.67 ATOM 1852 C VAL 1088 ATOM 1853 O VAL 1088 47,897 16,387 10,618 1,00 15,00 ATOM 1854 N TRP 1089 49,618 16,668 12,015 1,00 12,30 49.301 15.460 12.748 1.00 12.96 ATOM 1856 CA TRP 1089 50.236 15.279 13.960 1.00 16.98 ATOM 1857 CB TRP 1089 49.764 14.195 14.887 1.00 18.14 ATOM 1858 CG TRP 1089 50.325 12.884 15.031 1.00 18.48 49.476 12.162 15.893 1.00 20.05 ATOM 1859 CD2 TRP 1089 ATOM 1860 CE2 TRP 1089 ATOM 1861 CE3 TRP 1089 51,460 12,245 14,503 1.00 22,61 48.640 14.215 15.657 1.00 18.89 ATOM 1862 CD1 TRP 1089 48.451 12.995 16.255 1.00 19.54 ATOM 1863 NE1 TRP 1089 49,725 10,839 16,249 1,00 20,08 ATOM 1865 CZ2 TRP 1089 51.709 10.927 14.855 1.00 17.00 ATOM 1866 CZ3 TRP 1089 50.846 10.243 15,722 1.00 23.71 ATOM 1867 CH2 TRP 1089 47.873 15.711 13.207 1.00 14.68 ATOM 1868 C TRP 1089 46.987 14.958 12.842 1.00 20.33 ATOM 1869 O TRP 1089 47.636 16.823 13.923 1.00 18.59 ATOM 1870 N SER 1090 46.287 17.209 14.413 1.00 15.54 ATOM 1872 CA SER 1090 ATOM 1873 CB SER 1090 46,297 18,603 15,043 1.00 12.20 45.256 17.190 13.309 1.00 16.50 47.066 18.621 16.237 1.00 18.86 ATOM 1874 OG SER 1090 ATOM 1876 C SER 1090 ATOM 1877 O SER 1090 ATOM 1878 N PHE 1091 45,635 17,745 12,158 1,00 23,35 44.746 17.776 10.997 1.00 20.78 45.445 18.399 9.786 1.00 17.07 ATOM 1880 CA PHE 1091 ATOM 1881 CB PHE 1091 44.533 18.524 8.598 1.00 21.98 43.396 19.347 8.666 1.00 17.34 ATOM 1882 CG PHE 1091 ATOM 1883 CD1 PHE 1091 44,740 17.754 7.460 1.00 19.42 42.485 19.398 7.641 1.00 15.43 ATOM 1884 CD2 PHE 1091 ATOM 1885 CE1 PHE 1091 43.829 17.792 6.421 1.00 18.06 ATOM 1886 CE2 PHE 1091 42.693 18.618 6.509 1.00 19.76 ATOM 1887 CZ PHE 1091 42.693 18.616 0.507 1.00 17.25 44.306 16.332 10.667 1.00 17.25 ATOM 1888 C PHE 1091

## FIG. 7(38)

ATOM 1889 O PHE 1091 43.147 16.077 10.334 1.00 15.79 45.258 15.408 10.812 1.00 19.49 ATOM 1890 N GLY 1092 ATOM 1892 CA GLY 1092 45,042 13,988 10,577 1,00 18,11 ATOM 1893 C GLY 1092 44.029 13.429 11.544 1.00 19.35 ATOM 1894 O GLY 1092 43,235 12.581 11.137 1.00 24.23 44,073 13.836 12.819 1.00 18.53 ATOM 1895 N VAL 1093 43,055 13,392 13,788 1,00 20,09 ATOM 1897 CA VAL 1093 43.389 13.752 15.298 1.00 15.18 42.421 13.051 16.187 1.00 17.08 ATOM 1898 CB VAL 1093 ATOM 1899 CG1 VAL 1093 44,778 13,310 15,698 1.00 11,27 ATOM 1900 CG2 VAL 1093 ATOM 1901 C VAL 1093 41.661 13.971 13.376 1.00 22.42 ATOM 1902 O VAL 1093 40.649 13.253 13.396 1.00 26.19 41.618 15.235 12.938 1.00 23.95 ATOM 1903 N LEU 1094 40.363 15.893 12.484 1.00 19.63 ATOM 1905 CA LEU 1094 40.667 17.338 12.050 1.00 25.24 39.587 18.420 11.974 1.00 27 30 ATOM 1906 CB LEU 1094 ATOM 1907 CG LEU 1094 40.136 19.497 11.113 1.00 28.26 ATOM 1908 CD1 LEU 1094 38.265 17.929 11.385 1.00 27.54 ATOM 1909 CD2 LEU 1094 39.775 15.146 11.280 1.00 16.12 ATOM 1910 C LEU 1094 38,555 15,002 11,129 1,00 16,14 ATOM 1911 O LEU 1094 40.631 14.766 10.348 1.00 16.30 40.155 14.003 9.195 1.00 17.98 41.321 13.538 8.317 1.00 16.52 40.631 14.766 10.348 1.00 16.30 ATOM 1912 N LEU 1095 ATOM 1914 CA LEU 1095 ATOM 1915 CB LEU 1095 41.981 14.536 7.386 1.00 14.88 ATOM 1916 CG LEU 1095 42.807 13.734 6.399 1.00 11.81 ATOM 1917 CD1 LEU 1095 ATOM 1918 CD2 LEU 1095 40.931 15.401 6.639 1.00 21.08 39.437 12.770 9.722 1.00 17.52 ATOM 1919 C LEU 1095 38.324 12.448 9.270 1.00 16.23 ATOM 1920 O LEU 1095 40.077 12.105 10.697 1.00 14.50 39.509 10.916 11.304 1.00 14.02 ATOM 1921 N TRP 1096 ATOM 1923 CA TRP 1096 40.452 10.330 12.337 1.00 13.21 ATOM 1924 CB TRP 1096 40.010 8.992 12.850 1.00 18.93 ATOM 1925 CG TRP 1096 ATOM 1926 CD2 TRP 1096 39.016 8.732 13.856 1.00 24.77 ATOM 1927 CE2 TRP 1096 38,952 7.319 14.020 1.00 27.07 38.178 9.546 14.647 1.00 29.39 ATOM 1928 CE3 TRP 1096 40,483 7.781 12.460 1.00 21.28 39.854 6.770 13.154 1.00 18.61 38.075 6.700 14.954 1.00 28.21 37.303 8.927 15.581 1.00 29.42 37.266 7.511 15.719 1.00 27.60 ATOM 1929 CD1 TRP 1096 ATOM 1930 NE1 TRP 1096 ATOM 1932 CZ2 TRP 1096 ATOM 1933 CZ3 TRP 1096 ATOM 1934 CH2 TRP 1096

#### FIG. 7(39)

ATOM 1935 C TRP 1096 38.159 11.236 11.927 1.00 18.94 37.212 10.439 11.826 1.00 22.31 ATOM 1936 O TRP 1096 38.046 12.385 12.592 1.00 23.97 ATOM 1937 N GLU 1097 36.754 12.750 13.195 1.00 21.61 ATOM 1939 CA GLU 1097 36,823 14,012 14,041 1,00 26,60 ATOM 1940 CB GLU 1097 37.880 14.065 15.109 1.00 21.55 ATOM 1941 CG GLU 1097 37,795 15,380 15,800 1,00 23,56 ATOM 1942 CD GLU 1097 ATOM 1943 OE1 GLU 1097 36,726 15,591 16,393 1,00 21,97 ATOM 1944 OE2 GLU 1097 38.741 16.208 15.706 1.00 20.79 ATOM 1945 C GLU 1097 35.744 13.010 12.116 1.00 19.15 34.549 12.766 12.304 1.00 28.35 ATOM 1946 O GLU 1097 36,190 13,565 11,001 1,00 17,99 ATOM 1947 N ILE 1098 ATOM 1949 CA ILE 1098 35.244 13.821 9.915 1.00 17.98 35.862 14.650 8.732 1.00 13.59 ATOM 1950 CB ILE 1098 ATOM 1951 CG2 ILE 1098 34.880 14.725 7.568 1.00 13.47 ATOM 1952 CG1 ILE 1098 36,169 16,074 9,181 1,00 11,46 36.691 16.960 8.074 1.00 9.72 ATOM 1953 CD1 ILE 1098 34.645 12.529 9.372 1.00 16.07 ATOM 1954 C ILE 1098 33.444 12.445 9.171 1.00 18.22 ATOM 1955 O ILE 1098 ATOM 1956 N PHE 1099 35.460 11.499 9.171 1.00 20.11 ATOM 1958 CA PHE 1099 34,925 10,257 8,601 1,00 18,95 35,909 9,660 7.625 1.00 16.86 ATOM 1959 CB PHE 1099 ATOM 1960 CG PHE 1099 36,269 10,584 6,517 1,00 12,61 37.308 11.468 6.671 1.00 14.37 ATOM 1961 CD1 PHE 1099 35.522 10.624 5.362 1.00 18.03 ATOM 1962 CD2 PHE 1099 37.595 12.369 5.717 1.00 13.66 ATOM 1963 CE1 PHE 1099 ATOM 1964 CE2 PHE 1099 35.811 11.553 4.378 1.00 16.05 ATOM 1965 CZ PHE 1099 36.843 12.418 4.568 1.00 17.86 ATOM 1966 C PHE 1099 34,368 9,201 9,551 1,00 23,18 34.111 8.070 9.149 1.00 22.90 ATOM 1967 O PHE 1099 ATOM 1968 N SER 1100 34.274 9.553 10.825 1.00 26.68 33,652 8,690 11,820 1,00 24,51 ATOM 1970 CA SER 1100 ATOM 1971 CB SER 1100 34.504 8,572 13.079 1.00 25.60 ATOM 1972 OG SER 1100 34.826 9.842 13.625 1.00 29.76 ATOM 1974 C SER 1100 32,398 9,465 12,145 1,00 26,92 31.765 9.211 13.157 1.00 31.32 ATOM 1975 O SER 1100 32.018 40.387 11.251 1.00 28.15 ATOM 1976 N LEU 1101 30.860 11.241 11.453 1.00 24.97 ATOM 1978 CA LEU 1101 29.556 10.557 11.015 1.00 22.00 ATOM 1979 CB LEU 1101 29,423 10,410 9,495 1,00 25.66 ATOM 1980 CG LEU 1101

## FIG. 7(40)

ATOM	1981 CD1 LEU 1101	28.060 9.866 9.127 1.00 22.23
ATOM	1982 CD2 LEU 1101	29.632 11.768 8.829 1.00 32.30
ATOM	1983 C LEU 1101	30.771 11.779 12.888 1.00 26.64
ATOM	1984 O LEU 1101	29.793 11.552 13.580 1.00 31.34
ATOM	1985 N GLY 1102	31.828 12.446 13.336 1.00 24.93
ATOM	1987 CA GLY 1102	31.836 13.057 14.650 1.00 28.61
ATOM	1988 C GLY 1102	32.129 12.293 15.917 1.00 32.38
ATOM	1989 O GLY 1102	31.647 12.693 16.950 1.00 35.69
ATOM	1990 N ALA 1103	33.004 11.291 15.876 1.00 35.95
ATOM	1992 CA ALA 1103	33.354 10.500 17.060 1.00 31.27
ATOM	1993 CB ALA 1103	33.515 9.041 16.672 1.00 36.15
ATOM	1994 C ALA 1103	34.625 10.972 17.747 1.00 34.29
ATOM	1995 O ALA 1103	35.382 11.788 17.190 1.00 36.92
ATOM	1996 N SER 1104	34.886 10.417 18.934 1.00 33.11
ATOM	1998 CA SER 1104	36.087 10.744 19.715 1.00 35.13
ATOM	1999 CB SER 1104	35.906 10.422 21.207 1.00 38.40
ATOM	2000 OG SER 1104	34.719 10.964 21.765 1.00 50.36
ATOM	2002 C SER 1104	37,216 9.852 19.249 1.00 34.54
ATOM	2003 O SER 1104	37.039 8.640 19.167 1.00 33.44
ATOM	2004 N PRO 1105	38.395 10.434 18.963 1.00 32.93
ATOM	2005 CD PRO 1105	38.678 11.877 18.972 1.00 31.54
ATOM	2006 CA PRO 1105	39.571 9.693 18.513 1.00 29.88
ATOM	2007 CB PRO 1105	40.633 10.781 18.465 1.00 22.24
ATOM	2008 CG PRO 1105	39.883 11.965 18.079 1.00 28.04
ATOM	2009 C PRO 1105	39.919 8.659 19.582 1.00 32.54
ATOM	2010 O PRO 1105	39,480 8,795 20,731 1.00 28,79
ATOM	2011 N TYR 1106	40.700 7.648 19.196 1.00 34.52
ATOM	2013 CA TYR 1106	41.148 6.564 20.085 1.00 39.62
ATOM	2014 CB TYR 1106	42.374 6.994 20.896 1.00 37.66
ATOM	2015 CG TYR 1106	43.496 7.566 20.059 1.00 39.50
ATOM	2016 CD1 TYR 1106	43.690 8.957 19.976 1.00 37.50
ATOM	2017 CE1 TYR 1106	44.655 9.518 19.143 1.00 35.61
ATOM	2018 CD2 TYR 1106	44,315 6.739 19.293 1.00 34.54
ATOM	2019 CE2 TYR 1106	45.305 7.290 18.446 1.00 38.80
ATOM	2020 CZ TYR 1106	45.466 8.686 18.373 1.00 38.23
ATOM	2021 OH TYR 1106	46.412 9.240 17.520 1.00 31.37
ATOM	2023 C TYR 1106	40.022 6.128 21.016 1.00 47.24
ATOM	2024 O TYR 1106	40.100 6.296 22.247 1.00 46.94
ATOM	2025 N PRO 1107	38.947 5.570 20.431 1.00 52.30
ATOM	2026 CD PRO 1107	38.880 5.234 18.996 1.00 52.76

# FIG. 7(41)

ATOM	2027 CA PRO 1107	37.750	5.088 21.125 1.00 55.67
ATOM	2028 CB PRO 1107	37.078	4.223 20.066 1.00 55.09
ATOM	2029 CG PRO 1107	37.420	4.931 18.797 1.00 52.62
ATOM	2030 C PRO 1107	38.035	4.300 22.408 1.00 60.55
ATOM	2031 O PRO 1107	38.668	3.231 22.377 1.00 60.88
ATOM	2032 N GLY 1108	37.631	4.894 23.533 1.00 62.85
ATOM	2034 CA GLY 1108	37.790	4.284 24.845 1.00 63.10
ATOM	2035 C GLY 1108	39.171	3.783 25.228 1.00 61.44
ATOM	2036 O GLY 1108	39.319	3.010 26.178 1.00 63.49
ATOM	2037 N VAL 1109	40.181	4.228 24.498 1.00 58.31
ATOM	2039 CA VAL 1109	41.548	3.835 24.766 1.00 55.54
ATOM	2040 CB VAL 1109	42.430	4.181 23.580 1.00 54.11
ATOM	2041 CG1 VAL 1109	43.857	3.787 23.857 1.00 51.33
ATOM	2042 CG2 VAL 1109	41.875	3.528 22.306 1.00 54.09
ATOM	2043 C VAL 1109	42.006	4.657 25.949 1.00 57.04
ATOM	2044 O VAL 1109	41.492	5.749 26.163 1.00 57.18
ATOM	2045 N LYS 1110	42.969	4.140 26.711 1.00 59.43
ATOM	2047 CA LYS 1110	43.497	4.849 27.880 1.00 60.27
ATOM	2048 CB LYS 1110	43.928	3.842 28.936 1.00 63.70
ATOM	2049 C LYS 1110	44.664	5.796 27.538 1.00 60.52
ATOM	2050 O LYS 1110	45.570	5.410 26.780 1.00 61.06
ATOM	2051 N ILE 1111	44.665	7.006 28.115 1.00 58.79
ATOM	2053 CA ILE 1111	45.732	7.987 27.859 1.00 60.01
ATOM	2054 CB ILE 1111	45.236	9.441 27.886 1.00 63.41
ATOM	2055 CG2 ILE 1111	44.517	9.798 26.596 1.00 58.31
<b>ATOM</b>	2056 CG1 ILE 1111	44.413	9.688 29.145 1.00 69.87
ATOM	2057 CD1 ILE 1111	44.341	11.144 29.528 1.00 75.64
ATOM	2058 C ILE 1111	46.949	7.891 28.781 1.00 58.91
<b>ATOM</b>	2059 O ILE 1111	47.670	8.862 28.992 1.00 59.56
ATOM	2060 N ASP 1112	47.187	6.697 29.299 1.00 60.43
ATOM	2062 CA ASP 1112	48.312	6.407 30.173 1.00 56.25
ATOM	2063 CB ASP 1112	48.318	4.919 30.421 1.00 59.88
ATOM	2064 CG ASP 1112	48.273	4.131 29.122 1.00 67.87
ATOM	2065 OD1 ASP 1112	47.179	3.893 28.564 1.00 71.34
ATOM	2066 OD2 ASP 1112	49.348	3.765 28.628 1.00 72.11
ATOM	2067 C ASP 1112	49.612	6.795 29.489 1.00 54.37
ATOM	2068 O ASP 1112	49.634	
ATOM	2069 N GLU 1113	50.710	
ATOM	2071 CA GLU 1113	52.024	
ATOM	2072 CB GLU 1113	53.051	7.374 30.806 1.00 58.69

## FIG. 7(42)

52.552 6.015 28.726 1.00 54.42 ATOM 2073 C GLU 1113 53.624 6.175 28.126 1.00 51.91 51.822 4.903 28.627 1.00 51.54 52.192 3.819 27.719 1.00 54.36 51.873 2.452 28.322 1.00 56.43 53.072 1.749 28.948 1.00 63.29 53.996 2.661 29.772 1.00 67.36 55.153 2.870 29.329 1.00 67.36 ATOM 2074 O GLU 1113 ATOM 2075 N GLU 1114 ATOM 2077 CA GLU 1114 ATOM 2078 CB GLU 1114 ATOM 2079 CG GLU 1114 ATOM 2080 CD GLU 1114 ATOM 2081 OE1 GLU 1114 ATOM 2082 OE2 GLU 1114 53.590 3.127 30.873 1.00 68.20 ATOM 2083 C GLU 1114 51.440 4.031 26.412 1.00 52.22 51.830 3.514 25.360 1.00 51.74 ATOM 2084 O GLU 1114 ATOM 2085 N PHE 1115 50.383 4.840 26.486 1.00 49.67 ATOM 2087 CA PHE 1115 49.603 5.175 25.320 1.00 44.59 ATOM 2088 CB PHE 1115 48.400 6.013 25.688 1.00 44.73 ATOM 2089 CG PHE 1115 47.918 6.890 24.579 1.00 49.93 ATOM 2090 CD1 PHE 1115 48.140 8.270 24.621 1.00 50.02 ATOM 2091 CD2 PHE 1115 47.251 6.344 23.477 1.00 53.38 47,704 9,098 23,577 1,00 52,88 ATOM 2092 CE1 PHE 1115 ATOM 2093 CE2 PHE 1115 46.805 7.158 22.425 1.00 51.00 ATOM 2094 CZ PHE 1115 47.033 8.535 22.474 1.00 54.64 50.582 5.981 24.507 1.00 46.08 ATOM 2095 C PHE 1115 50,929 5.572 23.402 1.00 47.48 51.127 7.047 25.101 1.00 43.91 52.109 7.898 24.404 1.00 45.79 52.473 9.113 25.247 1.00 44.47 51.129 9.723 26.295 1.00 64.10 53.392 7.140 24.019 1.00 46.03 ATOM 2096 O PHE 1115 ATOM 2097 N CYS 1116 ATOM 2099 CA CYS 1116 ATOM 2100 CB CYS 1116 ATOM 2101 SG CYS 1116 ATOM 2102 C CYS 1116 53.392 7.140 24.019 1.00 46.03 ATOM 2103 O CYS 1116 54.232 7.667 23.279 1.00 46.86 ATOM 2104 N ARG 1117 53.536 5.911 24.529 1.00 44.91 ATOM 2106 CA ARG 1117 54.688 5.069 24.237 1.00 41.89 ATOM 2108 CG ARG 1117 56.237 3.298 25.233 1.00 43.78 ATOM 2109 CD ARG 1117 56.189 1.905 25.856 1.00 47.09 ATOM 2110 NE ARG 1117 55.490 0.922 25.021 1.00 49.55 ATOM 2113 NH1 ARG 1117 54.329 0.337 25.336 1.00 51.59 ATOM 2116 NH2 ARG 1117 53.695 0.649 26.461 1.00 47.17 ATOM 2119 C ARG 1117 54.320 0.337 25.336 1.00 43.78 ATOM 2120 O ARG 1117 55.156 4.455 21.996 1.00 42.49 ATOM 2121 N ARG 1118 53.206 3.751 22.860 1.00 35.52 ATOM 2102 C CYS 1116

#### FIG. 7(43)

ATOM 2123 CA ARG 1118 52.745 3.072 21.649 1.00 36.78
ATOM 2124 CB ARG 1118 51.330 2.559 21.880 1.00 31.14
ATOM 2125 CG ARG 1118 51.216 1.675 23.068 1.00 34.41
ATOM 2126 CD ARG 1118 49.766 1.587 23.535 1.00 45.83
ATOM 2127 NE ARG 1118 48.897 0.750 22.693 1.00 53.41
ATOM 2129 CZ ARG 1118 47.564 0.658 22.826 1.00 55.58 ATOM 2130 NH1 ARG 1118 46.862 -0.144 22.025 1.00 56.70 ATOM 2133 NH2 ARG 1118
ATOM 2136 C ARG 1118
ATOM 2137 O ARG 1118
52.742 4.067 20.471 1.00 38.92
ATOM 2138 N LEU 1119
52.063 5.186 20.711 1.00 40.67
ATOM 2140 CA LEU 1119
51.012 6.295 19.779 1.00 36.71
ATOM 2141 CB LEU 1119
51.012 7.416 20.540 1.00 32.46
ATOM 2143 CD1 LEU 1119
51.014 7.016 20.540 1.00 25.91
ATOM 2144 CD2 LEU 1119
51.014 7.016 20.049 1.00 25.91
ATOM 2145 C LEU 1119
51.015 7.093 19.024 1.00 25.91
ATOM 2146 O LEU 1119
53.301 6.728 19.245 1.00 38.89
ATOM 2147 N LYS 1120
53.301 6.728 19.245 1.00 38.89
ATOM 2149 CA LYS 1120
55.649 7.152 19.640 1.00 41.56
ATOM 2151 CG LYS 1120
55.649 7.152 19.640 1.00 42.85
ATOM 2152 CD LYS 1120
57.467 8.670 20.467 1.00 52.51 ATOM 2133 NH2 ARG 1118 ATOM 2153 CE LYS 1120 ATOM 2154 NZ LYS 1120 ATOM 2158 C LYS 1120 ATOM 2159 O LYS 1120 ATOM 2160 N GLU 1121 ATOM 2162 CA GLU 1121 ATOM 2163 CB GLU 1121 ATOM 2164 CG GLU 1121 ATOM 2165 CD GLU 1121 ATOM 2166 OE1 GLU 1121 ATOM 2160 OEI GLU 1121 56.403 0.485 21.119 1.00 67.24 ATOM 2168 C GLU 1121 55.739 3.284 16.968 1.00 39.16 ATOM 2169 O GLU 1121 56.224 2.423 16.216 1.00 39.90 ATOM 2170 N GLY 1122 54.525 3.805 16.781 1.00 31.72 ATOM 2173 C GLY 1122 53.838 3.550 15.531 1.00 22.36 ATOM 2174 O GLY 1122 51.791 2.779 14.633 1.00 18.01

46.921 1.380 23.745 1.00 55.55 57.467 8.670 20.467 1.00 52.51 58.407 8.989 21.620 1.00 60.23 59.298 10.206 21.321 1.00 69.72 58.605 11.557 21.283 1.00 76.23 56.351 6.050 18.825 1.00 43.73 57.287 6.342 18.073 1.00 47.49 55.892 4.800 18.966 1.00 43.94 56.453 3.636 18.262 1.00 41.07 56.415 2.395 19.147 1.00 48.40 57.553 2.283 20.112 1.00 58.39 57.183 1.451 21.309 1.00 64.79 156.403 0.483 21.119 1.00 67.43 157.657 1.778 2.243 11.00 7.24

#### FIG. 7(44)

ATOM 2175 N THR 1123 51.918 2.946 16.860 1.00 16.84 ATOM 2177 CA THR 1123 50.535 2.502 16.989 1.00 22.17 ATOM 2178 CB THR 1123 50.209 2.144 18.469 1.00 29.75 ATOM 2179 OG1 THR 1123 51.148 1.174 18.971 1.00 31.60 48.794 1.587 18.591 1.00 31.44 ATOM 2181 CG2 THR 1123 ATOM 2182 C THR 1123 49,653 3,673 16,453 1,00 23,74 49.655 3.673 16.453 1.00 23.74
49.940 4.850 16.721 1.00 18.73
48.597 3.354 15.701 1.00 22.93
47.735 4.379 15.125 1.00 17.39
48.094 4.680 13.670 1.00 17.70
49.478 5.192 13.406 1.00 14.31
51.046 6.935 13.684 1.00 10.98
52.067 6.988 14.533 1.00 16.02
4 53.260 7.468 14.63 1.08 8.74 ATOM 2183 O THR 1123 ATOM 2184 N ARG 1124 ATOM 2186 CA ARG 1124 ATOM 2187 CB ARG 1124 ATOM 2188 CG ARG 1124 ATOM 2189 CD ARG 1124 ATOM 2190 NE ARG 1124 ATOM 2192 CZ ARG 1124 ATOM 2193 NH1 ARG 1124 ATOM 2196 NH2 ARG 1124
ATOM 2199 C ARG 1124
ATOM 2200 O ARG 1124
ATOM 2201 N MET 1125
ATOM 2196 NH2 ARG 1124
A6.085 2.698 15.022 1.00 20.38
ATOM 2201 N MET 1125
ATOM 2196 NH2 ARG 1124
A6.085 2.698 15.022 1.00 20.38
ATOM 2201 N MET 1125
ATOM 2196 NH2 ARG 1124
AG 1124
A ATOM 2199 C ARG 1124 43.943 4.570 15.023 1.00 21.15 43.943 4.570 15.023 1.00 23.81 43.158 5.870 15.012 1.00 16.88 42.783 6.397 16.380 1.00 17.08 41.656 7.825 16.270 1.00 25.19 42.908 9.123 15.776 1.00 17.02 43.604 3.789 13.749 1.00 29.80 44.998 3.033 12.748 1.00 23.27 ATOM 2203 CA MET 1125 ATOM 2204 CB MET 1125 ATOM 2205 CG MET 1125 ATOM 2206 SD MET 1125 ATOM 2207 CE MET 1125 ATOM 2208 C MET 1125 44.298 3.923 12.748 1.00 33.37 ATOM 2209 O MET 1125 ATOM 2210 N ARG 1126
ATOM 22110 N ARG 1126
ATOM 2212 CA ARG 1126
ATOM 2213 CB ARG 1126
ATOM 2214 CG ARG 1126
ATOM 2215 CD ARG 1126
ATOM 2216 NE ARG 1126
ATOM 2216 NE ARG 1126
ATOM 2218 CZ ARG 1126
ATOM 2218 CZ ARG 1126
ATOM 2218 CZ ARG 1126
ATOM 2219 NH1 ARG 1126
ATOM 2222 NH2 ARG 1126
ATOM 2225 C ARG 1126
ATOM 2225 C ARG 1126
ATOM 2225 C ARG 1126
ATOM 2226 O ARG 1126
ATOM 2236 O ARG 1126 40.706 4.117 12.380 1.00 34.88 40.760- 2.725 10.676 1.00 29.80 39.888 3.508 9.812 1.00 29.83 39.743 2.782 8.460 1.00 32.24 ATOM 2226 O ARG 1126 ATOM 2227 N ALA 1127 ATOM 2229 CA ALA 1127 ATOM 2230 CB ALA 1127

#### FIG. 7(45)

ATOM 2231 C ALA 1127 38.518 3.697 10.415 1.00 34.29 ATOM 2232 O ALA 1127 37.944 2.727 10.881 1.00 39.95 ATOM 2233 N PRO 1128 37.943 4.934 10.335 1.00 34.66 ATOM 2234 CD PRO 1128 38.477 6.142 9.685 1.00 35.04 ATOM 2235 CA PRO 1128 36.612 5.251 10.871 1.00 31.59 ATOM 2236 CB PRO 1128 36,511 6,776 10,669 1.00 32,56 ATOM 2237 CG PRO 1128 37.819 7.222 10.499 1.00 31.06 ATOM 2238 C PRO 1128 35,648 4,597 9,916 1.00 33.99 35.975 4.429 8.749 1.00 38.28 ATOM 2239 O PRO 1128 ATOM 2240 N ASP 1129 34.416 4.371 10.344 1.00 31.98 ATOM 2242 CA ASP 1129 33,425 3,728 9,489 1,00 34,11 32,157 3,432 10,277 1,00 29,91 ATOM 2243 CB ASP 1129 32,447 2,811 11,623 1,00 34,04 ATOM 2244 CG ASP 1129 33,519 2,172 11,805 1,00 35,22 ATOM 2245 OD1 ASP 1129 31.597 2.976 12.515 1.00 36.43 ATOM 2246 OD2 ASP 1129 ATOM 2247 C ASP 1129 33.061 4.360 8.158 1.00 35.75 ATOM 2248 O ASP 1129 32,441 3.699 7.312 1.00 38.26 ATOM 2249 N TYR 1130 33,444 5.613 7.925 1.00 32.58 33.056 6.200 6.649 1.00 34.86 ATOM 2251 CA TYR 1130 32.067 7.332 6.888 1.00 38.26 ATOM 2252 CB TYR 1130 30,996 6,960 7,889 1,00 37,51 ATOM 2253 CG TYR 1130 ATOM 2254 CD1 TYR 1130 31.208 7.153 9.245 1.00 36.44 30.249 6.853 10.148 1.00 40.00 ATOM 2255 CE1 TYR 1130 29.787 6.442 7.468 1.00 39.18 ATOM 2256 CD2 TYR 1130 28.813 6.143 8.360 1.00 34.53 ATOM 2257 CE2 TYR 1130 ATOM 2258 CZ TYR 1130 29,050 6,353 9,709 1,00 39,16 28.120 6.147 10.690 1.00 47.34 ATOM 2259 OH TYR 1130 34.136 6.657 5.732 1.00 34.80 ATOM 2261 C TYR 1130 33.853 7.257 4.694 1.00 27.05 ATOM 2262 O TYR 1130 35,388 6,414 6,108 1,00 37,58 ATOM 2263 N THR 1131 36.457 6.829 5.238 1.00 38.70 ATOM 2265 CA THR 1131 37,783 6.598 5.763 1.00 39.57 ATOM 2266 CB THR 1131 37.775 5.417 6.564 1.00 51.23 ATOM 2267 OG1 THR 1131 ATOM 2269 CG2 THR 1131 38.250 7.775 6.481 1.00 49.58 ATOM 2270 C THR 1131 36,476 6,071 3,955 1,00 38,19 ATOM 2271 O THR 1131 35,913 4,967 3,808 1,00 38,82 ATOM 2272 N THR 1132 37.297 6.649 3.104 1.00 31.58 ATOM 2274 CA THR 1132 37,638 6,148 1,836 1,00 27,37 ATOM 2275 CB THR 1132 37.591 7.302 0.887 1.00 18.06 36,274 7,366 0,348 1.00 29.75 ATOM 2276 OG1 THR 1132

#### FIG. 7(46)

ATOM 2278 CG2 THR 1132
ATOM 2279 C THR 1132
ATOM 2280 O THR 1132
ATOM 2281 N PRO 1133
ATOM 2281 N PRO 1133
ATOM 2282 CD PRO 1133
ATOM 2283 CA PRO 1133
ATOM 2284 CB PRO 1133
ATOM 2285 CG PRO 1133
ATOM 2286 C PRO 1133
ATOM 2287 O PRO 1133
ATOM 2287 O PRO 1133
ATOM 2287 O PRO 1134
ATOM 2290 CA GLU 1134
ATOM 2290 CA GLU 1134
ATOM 2291 CB GLU 1134
ATOM 2292 CG GLU 1134
ATOM 2295 OE2 GLU 1134
ATOM 2295 OE2 GLU 1134
ATOM 2296 C GLU 1134
ATOM 2296 C GLU 1134
ATOM 2297 O GLU 1134
ATOM 2298 N MET 1135
ATOM 2300 CA MET 1135
ATOM 2300 CA MET 1135
ATOM 2301 CB MET 1135
ATOM 2303 CR MET 1135
ATOM 2304 CE MET 1135
ATOM 2305 C MET 1135
ATOM 2306 C MET 1135
ATOM 2306 C MET 1135
ATOM 2307 N TYR 1136
ATOM 2300 CA TYPL 1136
ATOM 2307 S TYR 1136
ATOM 2308 C TYR 1136
ATOM 2307 S TYR 1136
ATOM 2309 CA TYR 1136
ATOM 2307 S TYR 1136
ATOM 2300 C T TYR 1136
ATOM 2307 S TYR 1136
ATOM 2307 S TYR 1136
ATOM 2309 C T TYR 1136
ATOM 2309 C T TYR 1136
ATOM 2309 C T TYR 1136 ATOM 2278 CG2 THR 1132 38.528 7.126 -0.161 1.00 32.09 ATOM 2307 N TYR 1136 41.836 7.448 4.445 1.00 20.30 ATOM 2309 CA TYR 1136 42.565 6.817 5.540 1.00 17.65 ATOM 2310 CB TYR 1136 42.082 5.394 5.832 1.00 21.89 ATOM 2311 CG TYR 1136 42.786 4.775 7.041 1.00 26.17
ATOM 2312 CD1 TYR 1136 42.702 5.353 8.325 1.00 20.81
ATOM 2313 CE1 TYR 1136 43.364 4.781 9.427 1.00 17.33
ATOM 2314 CD2 TYR 1136 43.554 3.612 6.900 1.00 26.03
ATOM 2315 CE2 TYR 1136 44.225 3.034 7.998 1.00 12.75 ATOM 2316 CZ TYR 1136
ATOM 2316 CZ TYR 1136
ATOM 2317 OH TYR 1136
ATOM 2319 C TYR 1136
ATOM 2320 O TYR 1136
ATOM 2321 N GLN 1137

44.124 3.615 9.245 1.00 16.64
44.791 2.999 10.281 1.00 17.57
44.077 6.847 5.267 1.00 14.28
44.077 6.847 5.267 1.00 14.28
44.079 6.693 4.022 1.00 12.55

## FIG. 7(47)

ATOM 2323 CA GLN 1137 45.903 6.777 3.758 1.00 16.34 46.218 6.412 2.325 1.00 18.36 47.702 6.654 1.945 1.00 21.79 48.613 5.655 2.561 1.00 14.21 48.416 4.469 2.381 1.00 22.64 ATOM 2324 CB GLN 1137 ATOM 2325 CG GLN 1137 ATOM 2326 CD GLN 1137 ATOM 2327 OE1 GLN 1137 49.571 6.111 3.344 1.00 18.97 ATOM 2328 NE2 GLN 1137 ATOM 2331 C GLN 1137 46,415 8,193 4,041 1,00 20,40 ATOM 2332 O GLN 1137 47.598 8.378 4.391 1.00 25.11 45.564 9.194 3.807 1.00 18.65 ATOM 2333 N THR 1138 45.939 10.568 4.068 1.00 15.52 44.921 11.507 3.538 1.00 19.97 ATOM 2335 CA THR 1138 ATOM 2336 CB THR 1138 ATOM 2337 OG1 THR 1138 44.797 11.257 2.144 1.00 18.74 45,381 12,939 3,722 1,00 21,70 ATOM 2339 CG2 THR 1138 ATOM 2340 C THR 1138 46.111 10.721 5.566 1.00 12.73 ATOM 2341 O THR 1138 47.067 11.344 6.010 1.00 18.83 45.233 10.118 6.352 1.00 9.32 45.402 10.151 7.809 1.00 12.25 44.295 9.349 8.480 1.00 13.21 ATOM 2342 N MET 1139 ATOM 2344 CA MET 1139 ATOM 2345 CB MET 1139 ATOM 2346 CG MET 1139 42,967 10,007 8.354 1.00 5.60 41.708 8.982 9.003 1.00 17.66 40.510 9.337 7.925 1.00 2.00 ATOM 2347 SD MET 1139 ATOM 2348 CE MET 1139 46,773 9,567 8,198 1,00 15,96 ATOM 2349 C MET 1139 47.573 10.237 8.855 1.00 17.30 47.058 8.333 7.770 1.00 15.29 48.357 7.735 8.081 1.00 14.20 ATOM 2350 O MET 1139 ATOM 2351 N LEU 1140 ATOM 2353 CA LEU 1140 48.542 6.409 7.326 1.00 6.27 47.511 5.373 7.745 1.00 15.42 47.656 4.103 6.927 1.00 8.64 ATOM 2354 CB LEU 1140 ATOM 2355 CG LEU 1140 ATOM 2356 CD1 LEU 1140 47.648 5.103 9.246 1.00 14.99 ATOM 2357 CD2 LEU 1140 ATOM 2358 C LEU 1140 49.518 8.684 7.751 1.00 17.20 50.552 8.691 8.442 1.00 18.73 ATOM 2359 O LEU 1140 49.396 9.413 6.644 1.00 20.16 ATOM 2360 N ASP 1141 50.442 10.374 6.229 1.00 19.52 50.139 10.963 4.851 1.00 20.89 50.228 9.942 3.772 1.00 25.01 ATOM 2362 CA ASP 1141 ATOM 2363 CB ASP 1141 ATOM 2364 CG ASP 1141 50.537 8.765 4.074 1.00 30.17 ATOM 2365 OD1 ASP 1141 49.994 10.321 2.624 1.00 26.42 ATOM 2366 OD2 ASP 1141 50.627 11.521 7.207 1.00 15.10 51.762 11.905 7.502 1.00 8.73 ATOM 2367 C ASP 1141 ATOM 2368 O ASP 1141 ATOM 2369 N CYS 1142 49.504 12.101 7.637 1.00 10.75

#### FIG. 7(48)

ATOM 2371 CA CYS 1142 ATOM 2372 CB CYS 1142 ATOM 2373 SG CYS 1142 ATOM 2374 C CYS 1142 ATOM 2375 O CYS 1142 ATOM 2379 CB TRP 1143 ATOM 2380 CG TRP 1143 ATOM 2381 CD2 TRP 1143 ATOM 2382 CE2 TRP 1143 ATOM 2383 CE3 TRP 1143 ATOM 2384 CD1 TRP 1143 ATOM 2385 NE1 TRP 1143 ATOM 2387 CZ2 TRP 1143 ATOM 2388 CZ3 TRP 1143 ATOM 2389 CH2 TRP 1143 ATOM 2390 C TRP 1143 ATOM 2391 O TRP 1143 ATOM 2392 N HIS 1144 ATOM 2394 CA HIS 1144 ATOM 2395 CB HIS 1144 ATOM 2396 CG HIS 1144 ATOM 2397 CD2 HIS 1144 ATOM 2398 ND1 HIS 1144 ATOM 2400 CE1 HIS 1144 ATOM 2401 NE2 HIS 1144 ATOM 2403 C HIS 1144 ATOM 2404 O HIS 1144 ATOM 2405 N GLY 1145 ATOM 2407 CA GLY 1145 ATOM 2408 C GLY 1145 ATOM 2409 O GLY 1145 ATOM 2410 N GLU 1146 ATOM 2412 CA GLU 1146 ATOM 2413 CB GLU 1146 ATOM 2414 CG GLU 1146 ATOM 2415 CD GLU 1146 ATOM 2416 OE1 GLU 1146 ATOM 2417 OE2 GLU 1146

49,516 13,196 8,590 1,00 13,88 48.110 13.776 8.739 1.00 17.83 47.414 14.574 7.291 1.00 17.66 50.042 12.717 9.961 1.00 15.52 50.545 13.513 10.734 1.00 16.31 ATOM 2376 N TRP 1143 49.883 11.424 10.266 1.00 20.06 ATOM 2378 CA TRP 1143 50.344 10.830 11.528 1.00 17.66 49.393 9.727 11.991 1.00 15.44 48.041 10.236 12.273 1.00 14.25 46.814 9.495 12.233 1.00 18.13 45,774 10,401 12,540 1,00 12,59 45,774 10,401 12,540 1,0012,59 46,490 8,143 11,966 1,00 16,02 47,710 11,514 12,605 1,00 7,90 46,355 11,618 12,768 1,00 13,52 44,425 10,012 12,592 1,00 8,83 45.155 7.755 12.017 1.00 11.61 44.133 8.691 12.327 1.00 16.83 51.765 10.281 11.442 1.00 23.22 52.208 9.507 12.298 1.00 27.31 52.510 10.722 10.440 1.00 24.48 53.876 10.280 10.299 1.00 26.08 54.495 10.859 9.023 1.00 19.25 55.791 10.214 8.654 1.00 18.57 56.923 10.003 9.374 1.00 14.60 56.016 9.657 7.415 1.00 19.61 57.231 9.133 7.387 1.00 19.99 57.803 9.332 8.562 1.00 15.04 54,710 10,671 11,542 1,00 32,65 54.626 11.795 12.031 1.00 31.70 55.541 9.734 12.016 1.00 37.26 56.393 9.970 13.168 1.00 31.32 57.251 11.212 13.001 1.00 35.04 57.372 11.989 13.942 1.00 38.42 57.915 11.373 11.852 1.00 34.51 58.735 12.577 11.598 1.00 34.51 59.871 12.303 10.627 1.00 37.16 61.093 11.742 11.292 1.00 50.26 61.186 10.243 11.110 1.00 54.17 61.158 9.509 12.125 1.00 55.25 61.280 9.804 9.938 1.00 59.09

#### FIG. 7(49)

ATOM 2418 C GLU 1146 57.910 13.742 11.052 1.00 36.46 ATOM 2419 O GLU 1146 57.378 13.665 9.934 1.00 35.72 ATOM 2420 N PRO 1147 57.861 14.868 11.791 1.00 34.09 58,490 15,147 13.099 1.00 33.72 ATOM 2421 CD PRO 1147 ATOM 2422 CA PRO 1147 57.082 16.020 11.336 1.00 29.77 57.446 17.196 12.351 1.00 27.86 ATOM 2423 CB PRO 1147 57,668 16,334 13,619 1,00 26,72 ATOM 2424 CG PRO 1147 ATOM 2425 C PRO 1147 57.436 16.417 9.922 1.00 27.04 56.559 16.784 9.158 1.00 30.21 ATOM 2426 O PRO 1147 58.698 16.255 9.551 1.00 22.56 ATOM 2427 N SER 1148 59,177 16,616 8,210 1,00 24,23 ATOM 2429 CA SER 1148 ATOM 2430 CB SER 1148 60,707 16,724 8,203 1,00 27,40 ATOM 2431 OG SER 1148 61.314 15.477 8.545 1.00 36.19 ATOM 2433 C SER 1148 58,743 15,674 7,101 1,00 21,41 ATOM 2434 O SER 1148 ATOM 2435 N GLN 1149 58,890 15,964 5,913 1,00 24,41 58.272 14.508 7.485 1.00 25.45 ATOM 2437 CA GLN 1149 57.831 13.547 6,497 1.00 26.28 58.224 12.142 6.946 1.00 32.79 59.705 11.907 6.958 1.00 25.96 60.279 12.196 5.622 1.00 32.77 ATOM 2438 CB GLN 1149 ATOM 2439 CG GLN 1149 ATOM 2440 CD GLN 1149 ATOM 2441 OE1 GLN 1149 59.765 11.744 4.591 1.00 36.63 61.312 13.007 5.604 1.00 37.86 ATOM 2442 NE2 GLN 1149 ATOM 2445 C GLN 1149 56.327 13.670 6.278 1.00 23.40 55,783 13,145 5,306 1,00 23,12 ATOM 2446 O GLN 1149 ATOM 2447 N ARG 1150 55.662 14.339 7.215 1.00 22.72 54.226 14.581 7.132 1.00 17.86 53.721 15.243 8.392 1.00 16.38 54.161 14.532 9.598 1.00 13.96 53.285 14.903 10.728 1.00 15.08 ATOM 2449 CA ARG 1150 ATOM 2450 CB ARG 1150 ATOM 2451 CG ARG 1150 ATOM 2452 CD ARG 1150 53.632 14.090 11.879 1.00 24.55 ATOM 2453 NE ARG 1150 ATOM 2455 CZ ARG 1150 54.066 14.564 13.040 1.00 27.63 ATOM 2456 NH1 ARG 1150 54.192 15.871 13.230 1.00 27.18 ATOM 2459 NH2 ARG 1150 54,423 13,717 13,991 1,00 29,34 ATOM 2462 C ARG 1150 54.025 15.559 6.008 1.00 16.82 ATOM 2463 O ARG 1150 54,913 16.382 5.715 1.00 13.09 52.873 15.464 5.320 1.00 18.01 51.793 14.453 5.320 1.00 6.32 -52.726 16.442 4.240 1.00 18.95 51.489 15.948 3.492 1.00 16.01 54.913 16,382 5.715 1.00 13.09 ATOM 2464 N PRO 1151 ATOM 2465 CD PRO 1151 ATOM 2466 CA PRO 1151 51.489 15.948 3.492 1.00 16.01 ATOM 2467 CB PRO 1151 50.726 15.092 4.520 1.00 10.59 ATOM 2468 CG PRO 1151

#### FIG. 7(50)

ATOM 2469 C PRO 1151 52.574 17.861 4.805 1.00 18.27 ATOM 2470 O PRO 1151 52.422 18.039 6.006 1.00 19.70 ATOM 2471 N THR 1152 52.763 18.860 3.958 1.00 19.16 52.604 20.251 4.366 1.00 14.92 ATOM 2473 CA THR 1152 ATOM 2474 CB THR 1152 53.511 21.138 3.560 1.00 13.80 ATOM 2475 OG1 THR 1152 53,146 21,080 2,163 1,00 17,02 54.918 20.697 3.764 1.00 5.40 ATOM 2477 CG2 THR 1152 51.196 20.571 3.979 1.00 13.16 ATOM 2478 C THR 1152 ATOM 2479 O THR 1152 50.682 19.905 3.084 1.00 19.18 ATOM 2480 N PHE 1153 50.561 21.572 4.599 1.00 14.62 49.176 21.910 4.224 1.00 12.87 ATOM 2482 CA PHE 1153 48.588 23.023 5.083 1.00 11.95 48.157 22.558 6.422 1.00 9.67 ATOM 2483 CB PHE 1153 ATOM 2484 CG PHE 1153 47.037 21.740 6.560 1.00 14.91 ATOM 2485 CD1 PHE 1153 ATOM 2486 CD2 PHE 1153 48.891 22.857 7.533 1.00 15.01 46.660 21.215 7.802 1.00 9.44 ATOM 2487 CEI PHE 1153 48,529 22,340 8,789 1,00 13,43 ATOM 2488 CE2 PHE 1153 47.405 21.513 8.913 1.00 8.41 ATOM 2489 CZ PHE 1153 49.073 22.253 2.750 1.00 16.98 ATOM 2490 C PHE 1153 48.078 21.927 2.114 1.00 21.60 ATOM 2491 O PHE 1153 ATOM 2492 N SER 1154 50.116 22.841 2.168 1.00 15.39 ATOM 2494 CA SER 1154 50.031 23.123 0.754 1.00 17.55 51.251 23.868 0.254 1.00 25.28 ATOM 2495 CB SER 1154 51.244 25.190 0.776 1.00 33.35 ATOM 2496 OG SER 1154 49.850 21.815 0.022 1.00 20.26 ATOM 2498 C SER 1154 ATOM 2499 O SER 1154 48,932 21.704 -0.798 1.00 23.74 ATOM 2500 N GLU 1155 50.670 20.808 0.347 1.00 19.47 ATOM 2502 CA GLU 1155 50.534 19.493 -0.307 1.00 16.55 ATOM 2503 CB GLU 1155 51.588 18.513 0.188 1.00 19.82 ATOM 2504 CG GLU 1155 52.932 18.773 -0.486 1.00 20.20 ATOM 2505 CD GLU 1155 54.128 18.210 0.249 1.00 23.11 ATOM 2506 OE1 GLU 1155 55.226 18.377 -0.312 1.00 35.76 ATOM 2507 OE2 GLU 1155 54,009 17.631 1.359 1.00 21.09 ATOM 2508 C GLU 1155 49.153 18.918 -0.107 1.00 16.59 ATOM 2509 O GLU 1155 48.548 18.414 -1.055 1.00 21.37 48.619 19.034 1.101 1.00 16.01 ATOM 2510 N LEU 1156 47.272 18.532 1.375 1.00 18.06 ATOM - 2512 CA LEU 1156-46,969 18,521 2,875 1,00 15,74 ATOM 2513 CB LEU 1156 ATOM 2514 CG LEU 1156 47.688 17.493 3.759 1.00 11.35 47,786 18,049 5,201 1,00 2,08 ATOM 2515 CD1 LEU 1156

## FIG. 7(51)

ATOM 2516 CD2 LEU 1156 46.927 16.150 3.708 1.00 14.36 ATOM 2516 CD2 LEU 1156
ATOM 2517 C LEU 1156
ATOM 2518 O LEU 1156
ATOM 2519 N VAL 1157
ATOM 2521 CA VAL 1157
ATOM 2522 CB VAL 1157
ATOM 2523 CG1 VAL 1157
ATOM 2524 CG2 VAL 1157
ATOM 2525 C VAL 1157
ATOM 2525 C VAL 1157
ATOM 2526 O VAL 1157 ATOM 2526 C VAL 1157
ATOM 2527 N GLU 1158
ATOM 2529 CA GLU 1158
ATOM 2529 CA GLU 1158
ATOM 2530 CB GLU 1158
ATOM 2531 CG GLU 1158
ATOM 2532 CD GLU 1158
ATOM 2533 OE1 GLU 1158
ATOM 2533 OE1 GLU 1158
ATOM 2534 OE2 GLU 1158
ATOM 253 ATOM 2533 OE1 GLU 1158
ATOM 2534 OE2 GLU 1158
ATOM 2535 C GLU 1158
ATOM 2536 O GLU 1158
ATOM 2537 N HIS 1159
ATOM 2539 CA HIS 1159
ATOM 2540 CB HIS 1159
ATOM 2541 CG HIS 1159
ATOM 2542 CD2 HIS 1159
ATOM 2543 ND1 HIS 1159
ATOM 2546 CEI HIS 1159
ATOM 2546 NE2 HIS 1159
ATOM 2546 NE2 HIS 1159
ATOM 2547 CHIS 1159
ATOM 2548 C HIS 1159 ATOM 2548 C HIS 1159 44.402 16.104 -2.391 1.00 21.56 ATOM 2549 O HIS 1159 43.741 15.311 -3.066 1.00 22.19 ATOM 2550 N LEU 1160 43.852 16.874 -1.456 1.00 20.25 ATOM 2550 N LEU 1160
ATOM 2552 CA LEU 1160
ATOM 2553 CB LEU 1160
ATOM 2553 CB LEU 1160
ATOM 2555 CG LEU 1160
ATOM 2555 CD1 LEU 1160
ATOM 2556 CD2 LEU 1160
ATOM 2556 CD2 LEU 1160
ATOM 2557 C LEU 1160
ATOM 2558 O LEU 1160
ATOM 2559 N GLY 1161
ATOM 2559 N GLY 1161
ATOM 2561 CA GLY 1161
ATOM 2562 C GLY 1161
ATOM 2562 C GLY 1161
ATOM 2563 C GLY 1161
ATOM 2563 C GLY 1161
ATOM 2564 C GLY 1161
ATOM 2564 C GLY 1161
ATOM 2565 C GLY 1161
ATOM 2568 C GLY 1161
ATOM 2569 C GLY 1161

#### FIG. 7(52)

ATOM 2563 O GLY 1161 ATOM 2564 N ASN 1162 ATOM 2566 CA ASN 1162 ATOM 2567 CB ASN 1162 ATOM 2568 CG ASN 1162 ATOM 2569 OD1 ASN 1162 ATOM 2570 ND2 ASN 1162 ATOM 2573 C ASN 1162 ATOM 2574 O ASN 1162 ATOM 2575 N LEU 1163 ATOM 2577 CA LEU 1163 ATOM 2578 CB LEU 1163 ATOM 2579 CG LEU 1163 ATOM 2580 CD1 LEU 1163 ATOM 2581 CD2 LEU 1163 ATOM 2582 C LEU 1163 ATOM 2583 O LEU 1163 ATOM 2584 N LEU 1164 ATOM 2586 CA LEU 1164 ATOM 2587 CB LEU 1164 ATOM 2588 CG LEU 1164 ATOM 2589 CD1 LEU 1164 ATOM 2590 CD2 LEU 1164 ATOM 2592 O LEU 1164 ATOM 2593 N GLN 1165 ATOM 2595 CA GLN 1165 ATOM 2596 CB GLN 1165 ATOM 2597 CG GLN 1165 ATOM 2598 CD GLN 1165 ATOM 2599 OE1 GLN 1165 ATOM 2600 NE2 GLN 1165 ATOM 2603 C GLN 1165 ATOM 2604 O GLN 1165 ATOM 2605 N ALA 1166 ATOM 2607 CA ALA 1166 ATOM 2608 CB ALA 1166 ATOM 2609 C ALA 1166 ATOM 2610 O ALA 1166 ATOM 2611 N ASN 1167 ATOM 2613 CA ASN 1167

40.295 17.526 -5.971 1.00 23.05 42,439 16,997 -5,520 1,00 21,49 42.428 15.854 -6.428 1.00 22.31 43.771 15.109 -6.427 1.00 22.34 44,904 15.888 -7.062 1.00 20.03 44,705 16,903 -7.701 1.00 28.17 46.117 15.401 -6.873 1.00 32.22 41.356 14.851 -5.969 1.00 23.05 40.570 14.378 -6.769 1.00 26.11 41,360 14,490 -4,688 1.00 21.05 40,405 13.523 -4.166 1.00 19.91 40,695 13.172 -2.689 1.00 19.18 41.675 12.042 -2.275 1.00 18.62 42,959 12,120 -3,020 1,00 24,35 41.983 12.043 -0.804 1.00 14.82 39.015 14.038 -4.331 1.00 19.71 38.110 13.318 -4.767 1.00 23.11 38.860 15.328 -4.121 1.00 25.91 37.533 15.941 -4.226 1.00 29.28 37.603 17.388 -3.726 1.00 31.25 36.348 18.176 -3.371 1.00 25.75 35,429 17,396 -2,435 1.00 31.52 7.018 15.866 -5.653 1.00 30.07 35,953 15,330 -5,903 1,00 32,61 37.810 16.344 -6.598 1.00 33.76 37.423 16.317 -8.003 1.00 39.95 38.451 17.048 -8.855 1.00 46.90 38.758 18.474 -8.480 1.00 49.81 39.874 19.024 -9.348 1.00 56.23 41.056 18.945 -8.997 1.00 55.97 39,508 19,536 -10,518 1.00 60.66 37.304 14.898 -8.554 1.00 39.33 36,652 14,685 -9.568 1.00 42.09 38.059 13.965 -7.988 1.00 36.82 37.994 12.586 -8.441 1.00 34.66 39.096 11.748 -7.814 1.00 32.78 36,640 12,103 -7.991 1.00 36.63 35,969 11,381 -8.713 1.00 39.47 36,226 12,532 -6,800 1.00 40.01 34,911 12,158 -6,264 1.00 42,40 36.640 12.103 -7.991 1.00 36.63 34.911 12.158 -6.264 1.00 42.40

# FIG. 7(53)

ATOM	2614 CB ASN 1167	34.641 12.878 -4.919 1.00 42.99
ATOM	2615 CG ASN 1167	33.354 12.409 -4.242 1.00 40.80
ATOM	2616 OD1 ASN 1167	32.306 13.046 -4.348 1.00 40.18
ATOM	2617 ND2 ASN 1167	33.436 11.294 -3.532 1.00 36.58
ATOM	2620 C ASN 1167	33.822 12.498 -7.299 1.00 41.88
ATOM	2621 O ASN 1167	32.837 11.789 -7.391 1.00 41.83
ATOM	2622 N ALA 1168	34.057 13.558 -8.085 1.00 45.09
ATOM	2624 CA ALA 1168	33.187 14.065 -9.160 1.00 46.02
ATOM	2625 CB ALA 1168	32.507 12.933 -9.929 1.00 45.92
ATOM	2626 C ALA 1168	32.181 15.123 -8.728 1.00 48.61
ATOM	2628 O ALA 1168	32.627 16.233 -8.363 1.00 50.20
ATOM	2629 O HOH 1	46.858 21.496 16.690 1.00 23.54
ATOM	2632 O HOH 2	49.904 21.605 17.271 1.00 36.65
ATOM	2635 O HOH 3	49.682 18.133 17.657 1.00 50.47
<b>ATOM</b>	2638 O HOH 4	56.606 19.394 15.202 1.00 25.28
ATOM	2641 O HOH 5	57.215 21.949 11.395 1.00 37.66
ATOM	2644 O HOH 6	56.082 25.850 12.933 1.00 34.63
ATOM	2647 O HOH 7	52.355 23.016 6.377 1.00 21.45
ATOM	2650 O HOH 8	51.153 27.376 4.088 1.00 29.93
ATOM	2653 O HOH 9	44.820 28.454 1.120 1.00 16.47
<b>ATOM</b>	2656 O HOH 10	46.377 38.321 5.198 1.00 31.93
ATOM	2659 O HOH 11	43.987 38.133 3.129 1.00 52.41
ATOM	2662 O HOH 12	53.321 40.451 6.702 1.00 31.88
ATOM	2665 O HOH 13	44.977 49.530 8.305 1.00 44.56
ATOM	2668 O HOH 14	44.379 43.338 7.798 1.00 31.72
ATOM	2671 O HOH 15	39.477 40.232 8.468 1.00 36.65
ATOM	2674 O HOH 16	41.987 36.751 10.646 1.00 23.26
ATOM	2677 O HOH 17	41.711 41.873 6.802 1.00 34.79
ATOM	2680 O HOH 18	29.514 24.656 18.739 1.00 31.43
ATOM	2683 O HOH 19	27.493 22.351 15.517 1.00 42.03
ATOM	2686 O HOH 20	24.345 20.097 15.325 1.00 24.92
ATOM	2689 O HOH 21	32.381 18.452 20.520 1.00 75.12
ATOM	2692 O HOH 22	31.071 8.282 19.507 1.00 31.68
ATOM	2695 O HOH 23	33.001 7.742 21.598 1.00 38.67
ATOM	2698 O HOH 24	34.802 6.439 18.667 1.00 34.24
ATOM	2701 O HOH 25	32.273 6.932 14.174 1.00 41.21
ATOM	2704 O HOH 26 -	34.059 5.245 12.870 1.00 49.30
ATOM	2707 O HOH 27	38.059 3.432 4.799 1.00 63.69
ATOM	2710 O HOH 28	41.089 1.841 4.421 1.00 42.86
ATOM	2713 O HOH 29	45.081 9.234 -0.557 1.00 39.97

#### FIG. 7(54)

47.301 11.215 1.271 1.00 58.47 ATOM 2716 O HOH 30 50.046 14.055 0.168 1.00 37.58 ATOM 2719 O HOH 31 54.425 8.937 4.821 1.00 36.74 ATOM 2722 O HOH 32 52,279 7,099 5,152 1,00 13,04 ATOM 2725 O HOH 33 34 53,025 7,510 7,740 1,00 25,53 ATOM 2728 O HOH 50.852 6.818 10.462 1.00 18.29 ATOM 2731 O HOH 35 ATOM 2734 O HOH 36 46,448 7,762 15.254 1.00 9.08 ATOM 2737 O HOH 37 47.326 3.930 20.460 1.00 34.16 ATOM 2740 O HOH 38 48.264 12.367 20.804 1.00 22.14 ATOM 2743 O HOH 39 44,276 8,193 24,312 1,00 40,52 ATOM 2746 O HOH 40 37,491 11,237 25,975 1,00 38,71 ATOM 2749 O HOH 41 37.592 13.565 23.164 1.00 44.55 ATOM 2752 O HOH 42 34.887 12.418 26.235 1.00 50.96 ATOM 2755 O HOH 43 24.823 15.933 17.377 1.00 33.72 23.302 7.532 7.049 1.00 57.56 ATOM 2758 O HOH 44 29.954 11.864 -3.109 1.00 38.05 ATOM 2761 O HOH 45 ATOM 2764 O HOH 46 42,099 3,812 18,044 1,00 40,12 ATOM 2767 O HOH 47 38.653 0.737 18.003 1.00.37.30 34.169 14.465 16.707 1.00 20.01 ATOM 2770 O HOH 48 . 37,055 32,622 16,570 1.00 31,20 ATOM 2773 O HOH 49 50 29.361 31.729 15.460 1.00 21.90 ATOM 2776 O HOH 25.866 31.495 10.192 1.00 24.50 ATOM 2779 O HOH 51 ATOM 2782 O HOH 52 23.411 32.276 10.616 1.00 68.85 22.135 37.404 8.648 1.00 40.22 ATOM 2785 O HOH 53 28.356 36.997 10.747 1.00 22.41 ATOM 2788 O HOH 54 55 29,650 33,190 8,897 1,00 31,98 ATOM 2791 O HOH ATOM 2794 O HOH 56 34,801 35,904 3,297 1,00 59,73 57 24.341 20.715 4.934 1.00 28.10 ATOM 2797 O HOH 37.439 20.236 25.832 1.00 33.07 ATOM 2800 O HOH 58 ATOM 2803 O HOH 32.675 51.977 19.122 1.00 33.52 59 32.722 54.003 14.118 1.00 25.01 ATOM 2806 O HOH 60 ATOM 2809 O HOH 61 29,691 54,769 22.004 1.00 27.32 ATOM 2812 O HOH 62 21.347 47.577 14.711 1.00 27.85 ATOM 2815 O HOH 63 25.640 44.257 7.516 1.00 24.71 24.686 40.916 3.785 1.00 55.13 ATOM 2818 O HOH 64 ATOM 2821 O HOH 33.825 48.721 10.105 1.00 39.11 65 39.855 54.415 18.247 1.00 50.97 ATOM 2824 O HOH 66 ATOM 2827 O HOH 67 36.001 50.053 7.081 1.00 68.99 37.973 50.651 5.331 1.00 32.12 ATOM 2830 O HOH 68 ATOM 2833 O HOH 69 40.220 53.227 6.506 1.00 15.02

# FIG. 7(55)

ATOM	2836 O	HOH	70	42.258 51.833 6.993 1.00 21.05
ATOM	2839 O	нон	71	36.813 55.217 13.035 1.00 46.29
ATOM	2842 O	нон	72	37.030 55.879 15.712 1.00 39.36
ATOM	2845 O	HOH	73	23.054 45.061 23.607 1.00 51.11
ATOM	2848 O	HOH	74	27.075 54.516 6.971 1.00 51.66
ATOM	2851 O	HOH	75	21.634 54.039 13.651 1.00 36.36
ATOM	2854 O	HOH	76	45.158 47.529 30.699 1.00 56.11
ATOM	2857 O	HOH	77	44,469 45.246 36.699 1.00 36.50
ATOM	2860 O	HOH	78	45.882 41.717 36.085 1.00 28.57
ATOM	2863 O	HOH	79	49.406 41.527 34.292 1.00 65.94
ATOM	2866 O	HOH	80	36.134 49.719 26.101 1.00 63.80
ATOM	2869 O	HOH	81	26.884 28.564 16.554 1.00 49.20
ATOM	2872 O	HOH	82	22.079 10.131 13.444 1.00 56.45
ATOM	2875 O	HOH	83	41,225 4.655 30.464 1.00 58.98
ATOM	2878 O	нон	84	47.309 1.568 10.326 1.00 21.69
ATOM	2881 O	HOH	85	56.613 18.335 6.527 1.00 33.97
ATOM	2884 O	HOH	86	56.196 16.855 3.275 1.00 47.24
ATOM	2887 O	HOH	87	54.826 22.813 0.598 1.00 33.50
ATOM	2890 O	HOH	88	52.962 21.915 -2.351 1.00 66.62
ATOM	2893 O	HOH	89	47,896 24,242 -3.714 1.00 40.99
ATOM	2896 O	HOH	90	40.295 22.360 25.551 1.00 39.81
ATOM	2899 O	HOH	91	40.188 3.202 15.661 1.00 45.97
ATOM	2902 O	нон	92	45.159 2.965 19.553 1.00 44.25
ATOM	2905 O	нон	93	36.591 7.772 23.374 1.00 68.23
ATOM	2908 O		94	34.274 5.197 22.878 1.00 51.62
ATOM	2911 O		95	41.935 7.033 29.073 1.00 63.23
ATOM	2914 0	нон	96	20.731 12.105 14.716 1.00 54.80
ATOM	2917 O		97	23.147 13.682 17.882 1.00 50.81
ATOM	2920 O		98	35,515 9,509 -3,558 1,00 56,70
ATOM	2923 O		99	38.933 9.503 -1.231 1.00 32.18
ATOM	2926 O		100	51.814 24.438 3.703 1.00 52.00
ATOM	2929 O		101	51.670 28.690 0.838 1.00 42.41
ATOM	2932 O		102	46.536 30.610 1.750 1.00 45.80
ATOM	2935 O		103	45.165 34.214 0.818 1.00 46.46
ATOM	2938 O		104	42.695 35.194 1.055 1.00 25.82
ATOM	2941 O		105	39.689 33.418 0.723 1.00 31.99
ATOM	2944 O		106	23.962 38.119 27.549 1.00 47.89
ATOM	2947 O		107 .	25.343 40.908 27.379 1.00 54.09
ATOM	2950 O		108	20.307 35.738 19.866 1.00 32.61
ATOM	2953 O	нон	109	28.085 54.303 18.810 1.00 61.58

# FIG. 7(56)

ATOM	2956 O	нон	110	29.849 56.131 16.966 1.00 37.29
ATOM	2959 O	HOH	111	31.503 58.023 14.735 1.00 46.45
ATOM	2962 O	HOH	112	35.212 55.981 10.499 1.00 92.07
ATOM	2965 O	нон	113	36.530 55.812 6.656 1.00 30.72
ATOM	2968 O	нон	114	50,045 41.251 26.059 1.00 82.26
ATOM	2971 O	нон	115	25.153 36.460 9.054 1.00 50.86
ATOM	2974 O	нон	116	31,749 32,705 15,359 1.00 30.04
ATOM	2977 O	нон	117	30.213 3.806 4.940 1.00 39.74
ATOM	2980 O	HOH	118	36.511 1.159 7.275 1.00 41.62
ATOM	2983 O	HOH	119	27.155 4.637 5.224 1.00 79.92
ATOM	2986 O	HOH	120	57.319 11.287 3.459 1.00 33.02
ATOM	2989 O	HOH	121	52.121 12.483 1.755 1.00 45.55
ATOM	2992 O	HOH	122	47.613 14.088 -5.021 1.00 41.01
ATOM	2995 O	HOH	123	57.550 26.628 16.551 1.00 30.62
ATOM	2998 O	HOH	124	32.338 10.125 23.559 1.00 35.48
ATOM	3001 O	HOH	125	31.065 5.698 3.273 1.00 42.74
ATOM	3004 O	HOH	126	32.603 4.523 1.410 1.00 33.30
ATOM	3007 O	HOH	127	34.394 2.617 4.702 1.00 42.12
ATOM	3010 O	HOH	128	37.961 10.373 -4.287 1.00 47.57
ATOM	3013 O	HOH	129	42.215 11.947 -6.970 1.00 45.13
ATOM	3016 O	HOH	130	46.307 8.952 -4.280 1.00 70.02
ATOM	3019 O	HOH	131	50.369 17.388 -3.277 1.00 42.22
ATOM	3022 O	HOH	132	47.231 21.866 22.930 1.00 50.84
ATOM	3025 O	HOH	133	45.362 17.669 27.147 1.00 48.06
ATOM	3028 O	HOH	134	27.005 23.141 18.124 1.00 49.65
ATOM	3031 O	нон	135	45.726 12.511 -6.453 1.00 45.31
ATOM	3034 O	нон	136	46,998 11.755 18.088 1.00 37.38
ATOM	3037 O	нон	137	39.706 37.699 9.894 1.00 40.71
ATOM	3040 O	нон	138	18.768 48.678 17.798 1.00 74.62
ATOM	3043 O	нон	139	43.641 47.080 26.762 1.00 44.64
ATOM	3046 O	нон	140	32.593 53.980 16.744 1.00 43.95
ATOM	3049 O	нон	141	34.726 55.568 14.399 1.00 45.86
ATOM	3052 O	нон	142	30.551 53.227 19.638 1.00 35.99
ATOM	3055 O	HOH	143	26.370 55.161 14.300 1.00 33.09
ATOM	3058 O	нон	144	24.547 55.803 6.815 1.00 58.70
ATOM	3061 O	нон	145	36.217 52.574 3.221 1.00 68.48
ATOM	3064 O	HOH	146	39.065 54.455 4.595 1.00 48.85
ATOM	3067 O	нон	147	45.130 40.725 5.433 1.00 62.58
ATOM	3070 O		148	33.453 43.988 7.386 1.00 41.59
ATOM	3073 O	HOH	149	36.626 45.045 6.144 1.00 54.04

## FIG. 7(57)

ATOM	3076 O	нон	150	19.458 36.977 14.386 1.00 56.50
ATOM	3079 O	нон	151	19.502 40.993 17.850 1.00 43.35
ATOM	3082 O	нон	152	39.793 38.257 27.760 1.00 63.31
ATOM	3085 O	нон	153	40.730 53.944 20.682 1.00 49.91
ATOM	3088 O	нон	154	45.371 49.402 5.710 1.00 41.53
ATOM	3091 O	нон	155	49.114 26.038 11.482 1.00 34.43
ATOM	3094 O	нон	156	54.085 28.403 10.828 1.00 28.60
ATOM	3097 O	нон	157	18.729 14.990 12.752 1.00 44.66
ATOM	3100 O	HOH	158	27.500 2.046 10.138 1.00 47.88
ATOM	3103 O	нон	159	23.505 7.763 16.082 1.00 45.49
ATOM	3106 O	HOH	160	38.101 22.326 23.406 1.00 43.42
ATOM	3109 O	HOH	161	36.788 33.961 0.261 1.00 59.95
ATOM	3112 O	HOH	162	19.380 27.777 6.595 1.00 56.29
ATOM	3115 0	HOH	163	33.583 33.343 17.339 1.00 68.25
ATOM	3118 O	HOH	164	43.221 53.467 17.853 1.00 62.89
ATOM	3121 O	HOH	165	28.154 41.110 29.042 1.00 61.19
ATOM	3124 O	HOH	166	44.877 47.914 12.583 1.00 21.27
<b>ATOM</b>	3127 O	нон	167	46.589 45.908 14.329 1.00 39.48
ATOM	3130 O	HOH	168	48.235 43.490 14.297 1.00 46.88
ATOM	3133 O	HOH	169	47.834 0.528 14.762 1.00 74.55
ATOM	3136 O	нон	170	48.711 -2.009 16.386 1.00 52.45
ATOM	3139 O	HOH	171	41.210 0.396 17.381 1.00 58.05
ATOM	3142 O	HOH	172	43.837 1.538 17.483 1.00 72.30
ATOM	3145 O	HOH	173	41.780 -2.478 14.396 1.00 47.15
ATOM	3148 O	HOH	174	31.466 11.699 21.418 1.00 45.99
ATOM	3151 O	нон	175	35.046 14.218 20.429 1.00 39.37
ATOM	3154 O	нон	176	22.639 26.143 4.324 1.00 36.80
ATOM	3157 O	HOH	177	26.114 24.452 6.028 1.00 31.04
ATOM	3160 O	HOH	178	28.927 30.687 4.252 1.00 41.38
ATOM	3163 O	HOH	179	23.899 6.610 18.621 1.00 56.43
ATOM	3166 O	HOH	180	53.386 11.969 4.493 1.00 39.86
ATOM	3169 O	HOH	181	30.051 43.727 0.910 1.00 47.97
ATOM	3172 O	HOH	182	31.659 49.099 8.149 1.00 52.84